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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 02	STN pricing information for 2008 now available
NEWS 3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 5	JAN 28	MARPAT searching enhanced
NEWS 6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS 9	FEB 08	STN Express, Version 8.3, now available
NEWS 10	FEB 20	PCI now available as a replacement to DPCI
NEWS 11	FEB 25	IFIREF reloaded with enhancements
NEWS 12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS 13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS 16	MAR 31	CA/CAplus and CASREACT patent number format for U.S. applications updated
NEWS 17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS 18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS 20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS 21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS 22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS 23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS 24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS 27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 28	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS 29	JUN 25	CA/CAplus and USPAT databases updated with IPC reclassification data
NEWS 30	JUN 30	AEROSPACE enhanced with more than 1 million U.S.

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                  patent records
 NEWS 31  JUN 30  EMBASE, EMBAL, and LEMBASE updated with additional
                  options to display authors and affiliated
                  organizations
 NEWS 32  JUN 30  STN on the Web enhanced with new STN AnaVist
                  Assistant and BLAST plug-in
 NEWS 33  JUN 30  STN AnaVist enhanced with database content from EPFULL

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:50:43 ON 14 JUL 2008

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 15:51:30 ON 14 JUL 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   13 JUL 2008  HIGHEST RN 1033821-28-1
DICTIONARY FILE UPDATES:  13 JUL 2008  HIGHEST RN 1033821-28-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

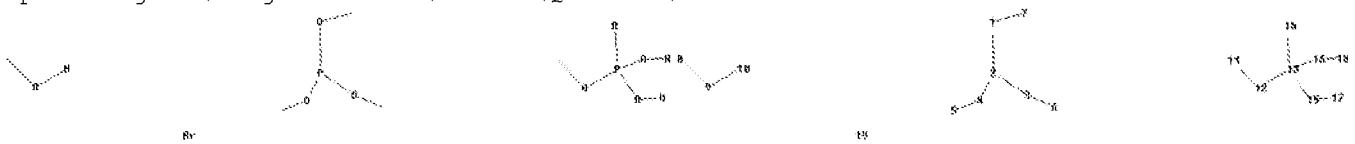
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.
```

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10587189.str



chain nodes :
1 2 3 4 9 10 12 13 14 15 16 17 18 19
ring/chain nodes :
5 6 7 8 11
chain bonds :
1-2 1-7 2-3 2-4 3-6 4-5 8-9 9-10 11-12 12-13 13-14 13-15 13-16 15-17
16-18
exact/norm bonds :
1-2 1-7 2-3 2-4 3-6 4-5 8-9 11-12 12-13 13-14 13-15 13-16
exact bonds :
9-10 15-17 16-18

Connectivity :
2:3 E exact RC ring/chain 13:4 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 19:CLASS
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
containing 8
containing 19
node mappings:
9:12 8:11 2:13

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> file casreact

```
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                          ENTRY    SESSION
FULL ESTIMATED COST                                        0.46       0.67

FILE 'CASREACT' ENTERED AT 15:51:48 ON 14 JUL 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 12 Jul 2008 VOL 149 ISS 3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*     CASREACT now has more than 13.8 million reactions    *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d l1
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 15:52:12 FILE 'CASREACT'
SCREENING COMPLETE -      821 REACTIONS TO VERIFY FROM       41 DOCUMENTS

100.0% DONE     821 VERIFIED      66 HIT RXNS                        6 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:     14702 TO    18138
PROJECTED ANSWERS:               6 TO      265

L2            6 SEA SSS SAM L1 (    66 REACTIONS)

=> d l2

L2   ANSWER 1 OF 6  CASREACT  COPYRIGHT 2008 ACS on STN

RX(9) OF 14 - REACTION DIAGRAM NOT AVAILABLE


=> d scan ti hit
```

```
INVALID SCAN FIELD FOR FILE 'CASREACT'

One or more of the display fields specified are not valid with DISPLAY
SCAN in the current file.  Enter HELP DSCAN at the arrow prompt (=>)
for the list of fields that may be used when scanning the answers.

=> D l1 ibib abs
L1 HAS NO ANSWERS
'IBIB ABS ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
          data.  (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
          data.
SDA ----- All Structure DAta (image, attributes, connection table and
          map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:sim
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> d l1 ibib abs hitstr
L1 HAS NO ANSWERS
'IBIB ABS HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
          data.  (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
          data.
SDA ----- All Structure DAta (image, attributes, connection table and
          map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:nos
L1              STR


=> d l1
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss full
FULL SEARCH INITIATED 15:57:19 FILE 'CASREACT'
SCREENING COMPLETE -     7766 REACTIONS TO VERIFY FROM      627 DOCUMENTS

100.0% DONE    7766 VERIFIED     472 HIT RXNS (     5 INCOMP)      45 DOCS
SEARCH TIME: 00.00.03

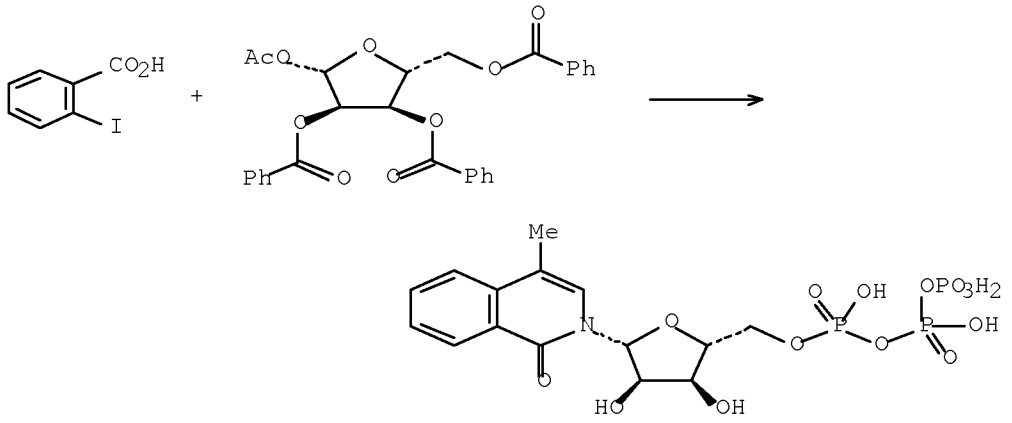
L3           45 SEA SSS FUL L1 (   472 REACTIONS)
```

=> d scan

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Novel nucleotide triphosphates as potent P2Y2 agonists

RX(42) OF 50 - 2 STEPS



NOTE: 2) analogues have similar reaction

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Total Synthesis of Geranylgeranylglyceryl Phosphate Enantiomers: Substrates for Characterization of 2,3-O-Digeranylgeranylglyceryl Phosphate Synthase

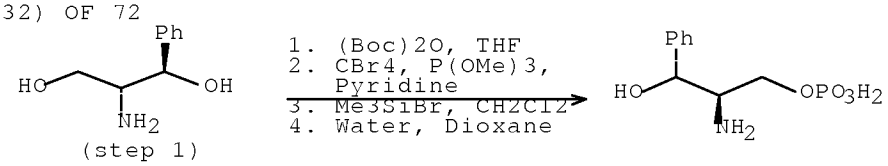
RX(16) OF 33 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis and biological properties of novel sphingosine derivatives

RX(32) OF 72



(step 1)

NOTE: regioselective stage 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI NBS-DMSO as a nonaqueous non-basic oxidation reagent for the synthesis of oligonucleotides

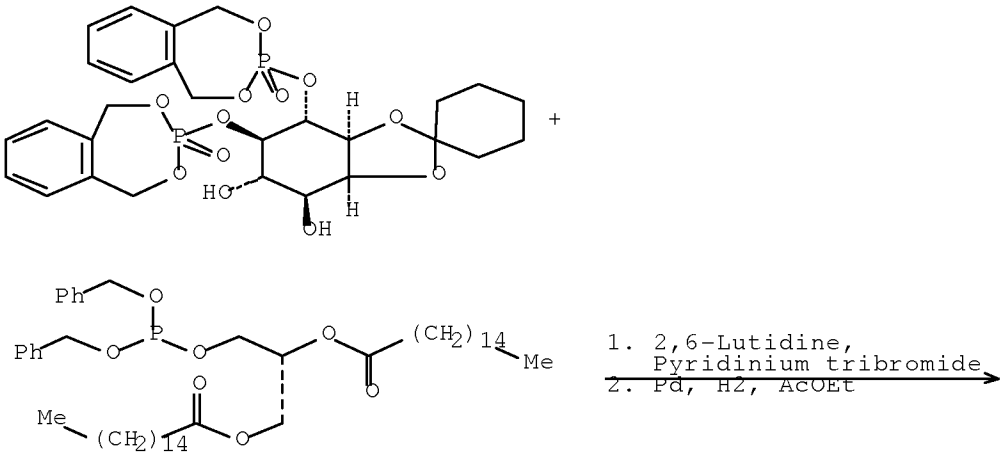
RX(33) OF 49 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

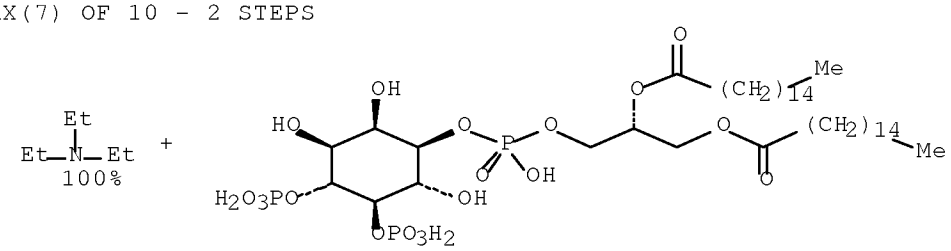
L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI A short synthesis of dipalmitoylphosphatidylinositol 4,5-bisphosphate via 3-O-selective phosphorylation of a 3,4-free inositol derivative

RX(7) OF 10 - 2 STEPS



RX(7) OF 10 - 2 STEPS

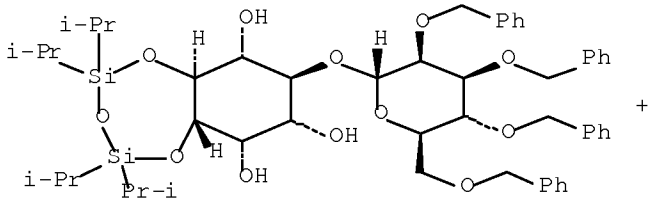


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

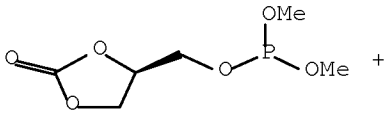
TI Regiospecific Synthesis of 2,6-Di-O-(α-D-mannopyranosyl)phosphatidyl-D-myo-inositol

RX(27) OF 29 - 5 STEPS



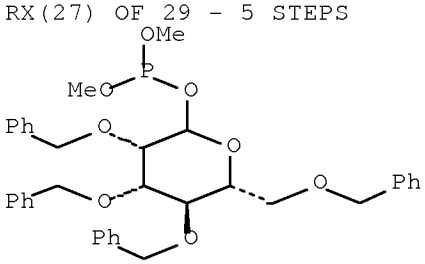
stereoisomers

+



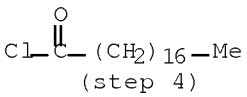
+

RX(27) OF 29 - 5 STEPS



(step 2)

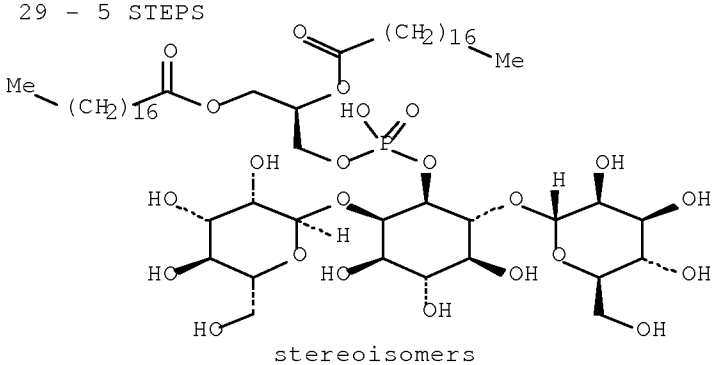
+



(step 4)

1. Pyridinium tribromide, Et3N, CH2Cl2
2. Me3SiSO3CF3
3. EtMgCl
4. Pyridine

RX(27) OF 29 - 5 STEPS



stereoisomers

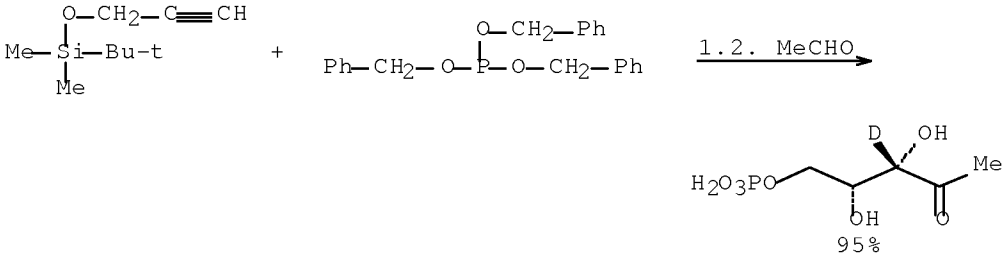
NOTE: 1) 83% overall, regioselective, 4) 73% OVERALL, 5) ISOMERIC REACTANTS ALSO PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI The chemical mechanism of D-1-deoxyxylulose-5-phosphate reductoisomerase from Escherichia coli

RX(85) OF 110 - 7 STEPS



95%

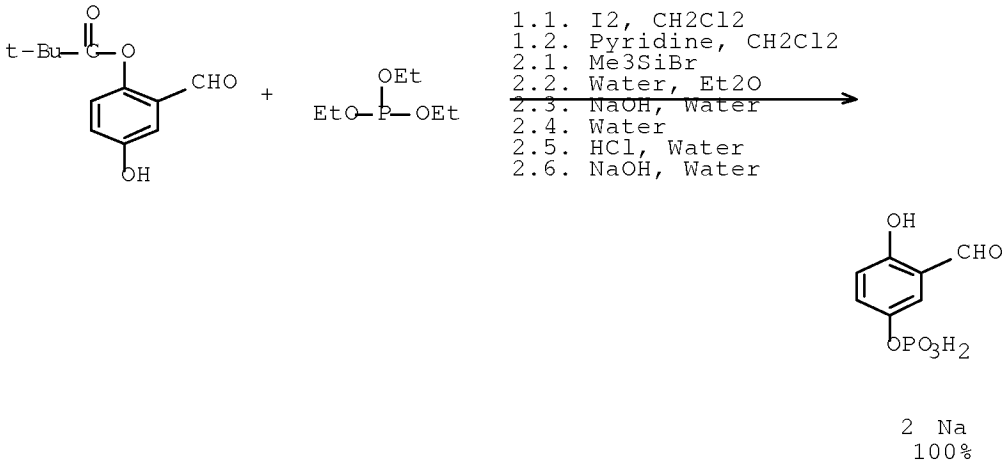
NOTE: 2) in-situ generated reagent (stage 1), regioselective, 4) regioselective, 5) Dess-Martin oxidation, 6) stereoselective

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Cell permeation of a Trypanosoma brucei aldolase inhibitor: Evaluation of different enzyme-labile phosphate protecting groups

RX(14) OF 42 - 2 STEPS



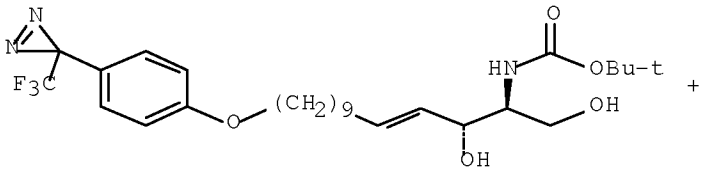
2 Na
100%

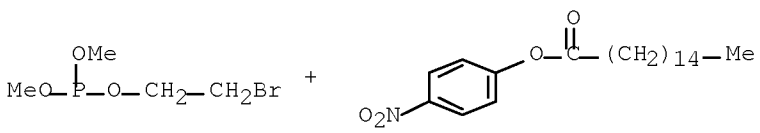
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Photoaffinity-labeled sphingomyelin analogs and processes thereof

RX(30) OF 53 - 3 STEPS

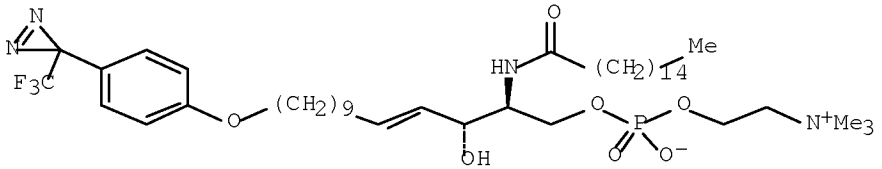




(step 2.2)

RX(30) OF 53 - 3 STEPS

1.1. CBr4, Pyridine
1.2. HCl, Water
2.1. F3CCO2H, CH2Cl2
2.2. Et3N, THF
3. Me3N, MeOH



71%

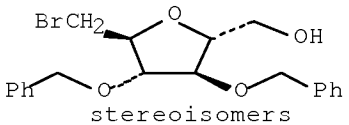
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan 1-45
'1-45' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

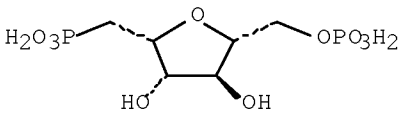
TI Synthesis of C-arabinofuranosyl compounds. Phosphonate and carboxylate isosteres of D-arabinose 1,5-bisphosphate

RX(71) OF 140 - 4 STEPS



stereoisomers

1. (PhO)2P(O)Cl, Pyridine, CH2Cl2
2. R:2161-16-2
3.1. Bu4NOH, THF
3.2. HCl, Water
4.1. Pd, H2, t-BuOH, Water
4.2. PtO2, H2, Water



NOTE: 1) 67% overall, 2) 16 h, 178.degree.

The following are valid formats:

```
ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
```

multistep reactions that have a hit substance in both
the first and last steps of the reaction, except for
those hit reactions whose steps are totally included
within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

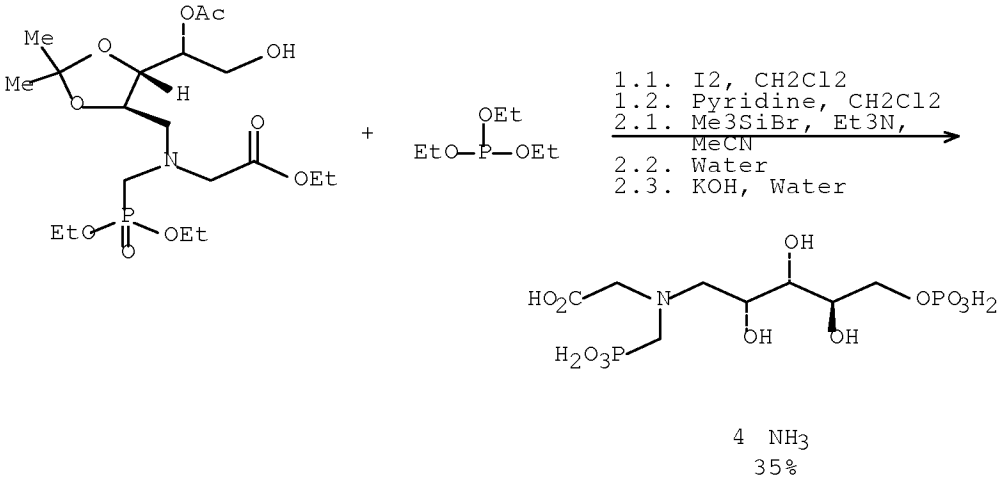
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan 1-45
'1-45' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis and evaluation of a mechanism-based inhibitor of a
3-deoxy-D-arabino heptulosonate 7-phosphate synthase

RX(17) OF 45 - 2 STEPS



The following are valid formats:

ABS -------- GI and AB
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APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications

ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

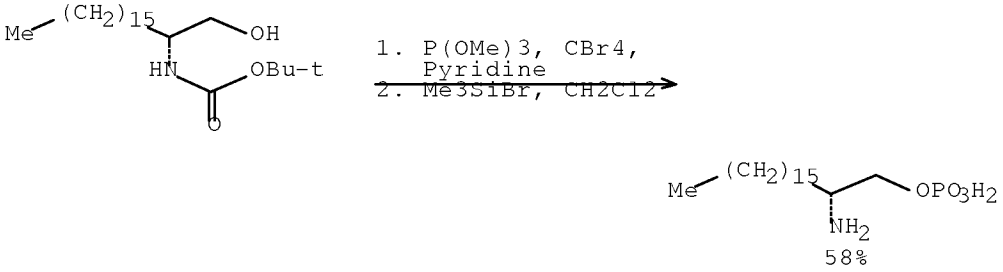
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Syntheses of sphingosine-1-phosphate analogues and their interaction with EDG/S1P receptors

RX(88) OF 285 - 2 STEPS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan ti hit
INVALID SCAN FIELD FOR FILE 'CASREACT'

One or more of the display fields specified are not valid with DISPLAY SCAN in the current file. Enter HELP DSCAN at the arrow prompt (=>) for the list of fields that may be used when scanning the answers.

=> d l3 ibib abs hitstr
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for

```
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>).  Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD.  The information is displayed in the same order
as the specification.  All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):
ENTER DISPLAY FORMAT (FCRDREF):o
'O' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
```

```
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed
```

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

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ENTER DISPLAY FORMAT (FCRDREF):fcrdfef
'FCRDFEF' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
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RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
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RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
```

path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):ti

L3 ANSWER 1 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
TI Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates

=> d l3 bib rx

L3 ANSWER 1 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
AN 148:79206 CASREACT Full-text
TI Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates
IN Lockwood, Samuel F.; Tang, Peng Cho; Nadolski, Geoff; Jackson, Henry L.; Fang, Zhiqiang; Du, Yishu; Yang, Min; Geiss, William; Williams, Richard; Burdick, David; Braun, Christi L.
PA Cardax Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 84pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007147163	A2	20071221	WO 2007-US71482	20070618
	WO 2007147163	A3	20080320		

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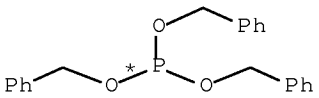
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRAI US 2006-814269P 20060616
OS MARPAT 148:79206

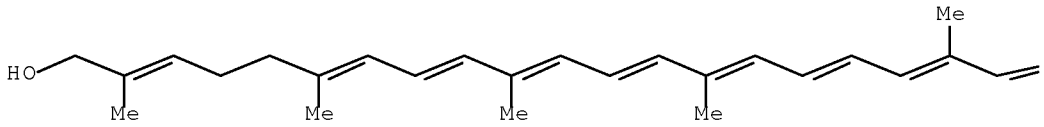
VERIFICATION INCOMPLETE - REACTION MAP DATA UNAVAILABLE

RX(127) OF 304 COMPOSED OF RX(18), RX(19), RX(20)
RX(127) AU + 4 AO ===> BG + BH



AU

PAGE 1-A



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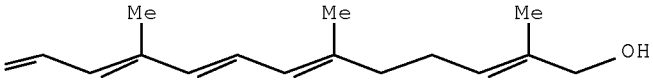
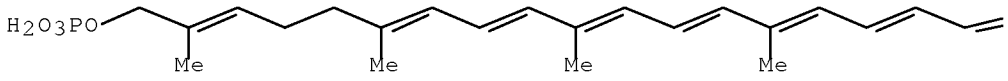


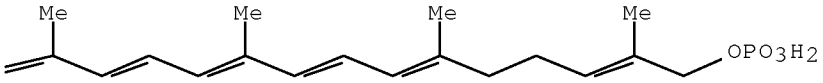
4 AO

3
STEPS

PAGE 1-A

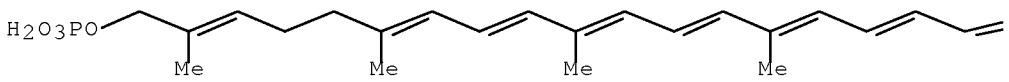


PAGE 1-B

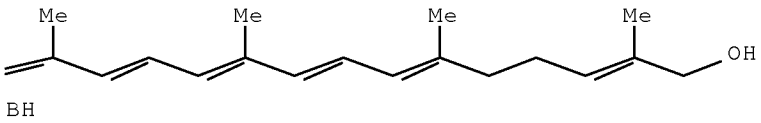


BG
YIELD 45%

PAGE 1-A



PAGE 1-B



RX(18) RCT AU 15205-57-9

STAGE(1)
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)
RGT AZ 7553-56-2 I2
CON SUBSTAGE(1) 10 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 10 minutes, room temperature

PRO AY 877774-61-3

RX(19) RCT AO 19891-75-9

STAGE(1)
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)
RGT BE 110-86-1 Pyridine
CON 0 deg C

STAGE(3)
RCT AY 877774-61-3
SOL 75-09-2 CH2Cl2
CON 1 hour, 0 deg C

STAGE(4)
SOL 75-09-2 CH2Cl2
CON 0 deg C

STAGE(5)
RGT BF 7647-14-5 NaCl
SOL 7732-18-5 Water
CON 0 deg C

PRO BA 882491-48-7, BB 914359-41-4, BC 882491-49-8D, BD 914359-40-3
NTE last stage quench

RX(20) RCT BA 882491-48-7, BB 914359-41-4, BC 882491-49-8D, BD 914359-40-3

STAGE(1)
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

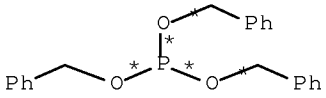
STAGE(2)
RGT BI 10416-59-8 Me3SiN:CMeOSiMe3
CON 0 deg C

STAGE(3)
RGT BJ 2857-97-8 Me3SiBr
CON 15 minutes, 0 deg C

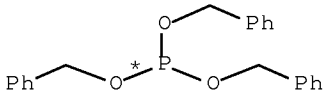
STAGE(4)
RGT AW 121-44-8 Et3N
CON 5 minutes, 0 deg C

PRO BG 882491-49-8, BH 914092-96-9
NTE fourth stage quench

RX(128) OF 304 COMPOSED OF RX(18), RX(19), RX(21)
RX(128) 5 AO + 4 AO ===> BK

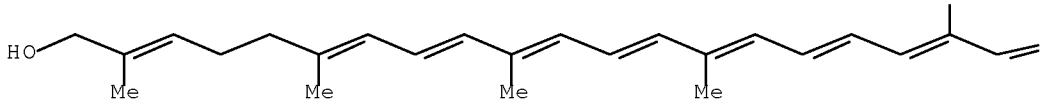


AU

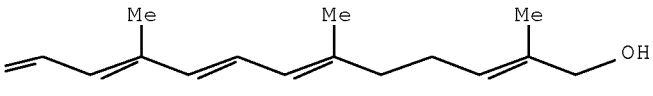


4 AU

PAGE 1-A



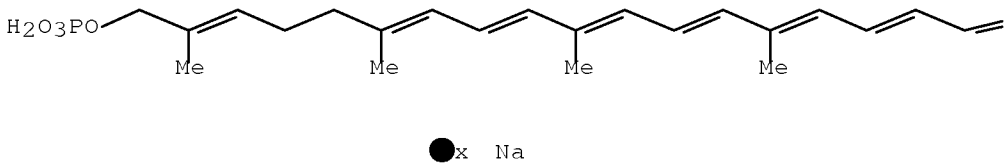
PAGE 1-B



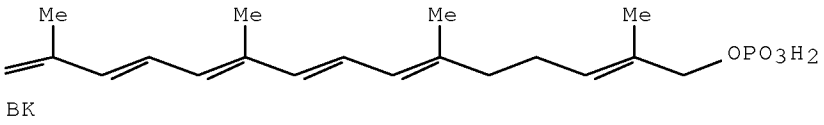
4 AO

3
STEPS

PAGE 1-A



PAGE 1-B



RX(18) RCT AU 15205-57-9

STAGE(1)
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)
RGT AZ 7553-56-2 I2
CON SUBSTAGE(1) 10 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 10 minutes, room temperature

PRO AY 877774-61-3

RX(19) RCT AO 19891-75-9

STAGE(1)
SOL 75-09-2 CH2Cl2
CON room temperature -> 0 deg C

STAGE(2)
RGT BE 110-86-1 Pyridine
CON 0 deg C

STAGE(3)
RCT AY 877774-61-3
SOL 75-09-2 CH2Cl2
CON 1 hour, 0 deg C

STAGE(4)
SOL 75-09-2 CH2Cl2
CON 0 deg C

STAGE(5)
RGT BF 7647-14-5 NaCl

```
                SOL  7732-18-5 Water
                CON  0 deg C

           PRO  BA 882491-48-7, BB 914359-41-4, BC 882491-49-8D, BD 914359-40-3
           NTE  last stage quench

RX(21)     RCT  BA 882491-48-7

             STAGE(1)
                RGT  BB 914359-41-4 ψ,ψ-Carotene-16,16'-diol,
                     16-(dihydrogen phosphate) 16'-(phenylmethyl hydrogen
                     phosphate), (1E,1'E)-, BC 882491-49-8D ψ,ψ-Carotene-
                     16,16'-diol, 16,16'-bis(dihydrogen phosphate), (1E,1'E)-,
                     BD 914359-40-3 ψ,ψ-Carotene-16,16'-diol,
                     16-[bis(phenylmethyl) phosphate] 16'-(phenylmethyl hydrogen
                     phosphate), (1E,1'E)-
                SOL  75-09-2 CH2Cl2
                CON  room temperature -> 0 deg C

             STAGE(2)
                RGT  BI 10416-59-8 Me3SiN:CMeOSiMe3
                CON  0 deg C

             STAGE(3)
                RGT  BJ 2857-97-8 Me3SiBr
                CON  15 minutes, 0 deg C

             STAGE(4)
                RGT  AW 121-44-8 Et3N
                CON  5 minutes, 0 deg C

             STAGE(5)
                SOL  67-56-1 MeOH
                CON  0 deg C

             STAGE(6)
                RGT  Q 124-41-4 NaOMe
                SOL  67-56-1 MeOH
                CON  SUBSTAGE(1) 0 deg C
                     SUBSTAGE(2) 0 deg C -> room temperature
                     SUBSTAGE(3) overnight, room temperature
                     SUBSTAGE(4) room temperature -> 0 deg C

             STAGE(7)
                SOL  7732-18-5 Water
                CON  5 minutes, 0 deg C

           PRO  BK 960203-78-5
           NTE  fourth stage quench




=> d scan ti

L3    45 ANSWERS   CASREACT  COPYRIGHT 2008 ACS on STN
TI   Synthesis of (R)-2-methyl-4-deoxy and (R)-2-methyl-4,5-dideoxy analogues
     of 6-phosphogluconate as potential inhibitors of 6-phosphogluconate
```

dehydrogenase

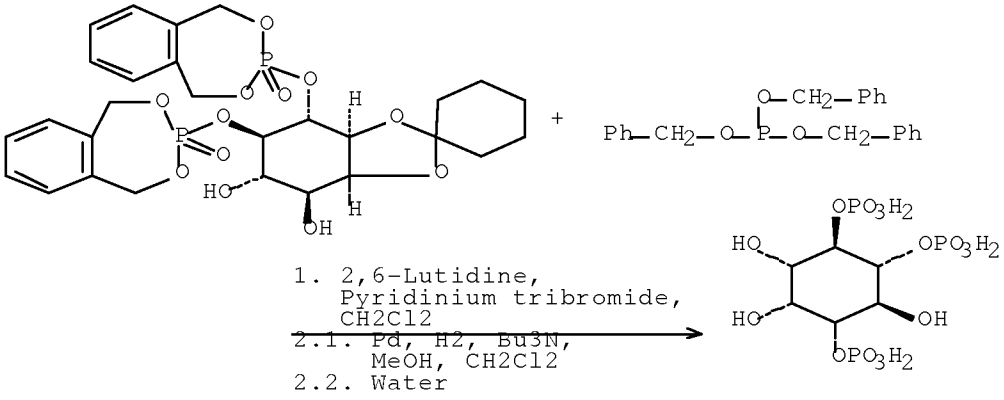
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan ti rxn
'RXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Regioselective phosphorylation of vicinal 3,4-hydroxy myo-inositol derivative promoted practical synthesis of d-PtdIns(4,5)P2 and D-Ins(1,4,5)P3

RX(21) OF 26 - 2 STEPS



3 Na
100%

NOTE: 1) regioselective, 2) Na+ and H+cation resin used in last stage

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN

```
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>).  Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD.  The information is displayed in the same order
as the specification.  All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

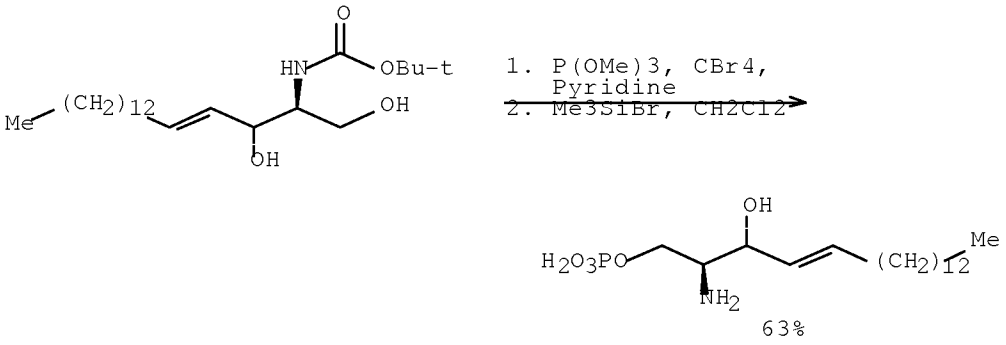
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan

L3   45 ANSWERS   CASREACT  COPYRIGHT 2008 ACS on STN

TI   Syntheses of sphingosine-1-phosphate stereoisomers and analogues and their
     interaction with EDG receptors
```

RX(18) OF 35 - 2 STEPS

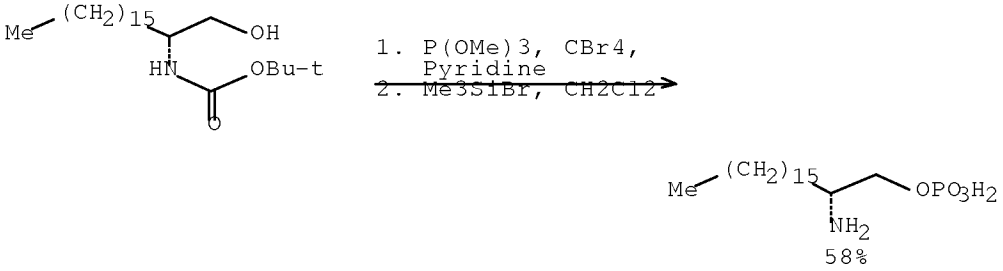


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Syntheses of sphingosine-1-phosphate analogues and their interaction with EDG/S1P receptors

RX(88) OF 285 - 2 STEPS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> d scan all
INVALID SCAN FIELD FOR FILE 'CASREACT'

One or more of the display fields specified are not valid with DISPLAY
SCAN in the current file.  Enter HELP DSCAN at the arrow prompt (=>)
for the list of fields that may be used when scanning the answers.

=> d his

     (FILE 'HOME' ENTERED AT 15:50:43 ON 14 JUL 2008)

     FILE 'REGISTRY' ENTERED AT 15:51:30 ON 14 JUL 2008
L1              STRUCTURE UPLOADED

     FILE 'CASREACT' ENTERED AT 15:51:48 ON 14 JUL 2008
L2            6 S L1
L3           45 S L1 SSS FULL

=> d ibib abs fcrd 1-
YOU HAVE REQUESTED DATA FROM 45 ANSWERS - CONTINUE? Y/(N):y
```

L3 ANSWER 1 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 148:79206 CASREACT Full-text
TITLE: Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates
INVENTOR(S): Lockwood, Samuel F.; Tang, Peng Cho; Nadolski, Geoff; Jackson, Henry L.; Fang, Zhiqiang; Du, Yishu; Yang, Min; Geiss, William; Williams, Richard; Burdick, David; Braun, Christi L.
PATENT ASSIGNEE(S): Cardax Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 84pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007147163	A2	20071221	WO 2007-US71482	20070618
WO 2007147163	A3	20080320		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2006-814269P 20060616
OTHER SOURCE(S): MARPAT 148:79206
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

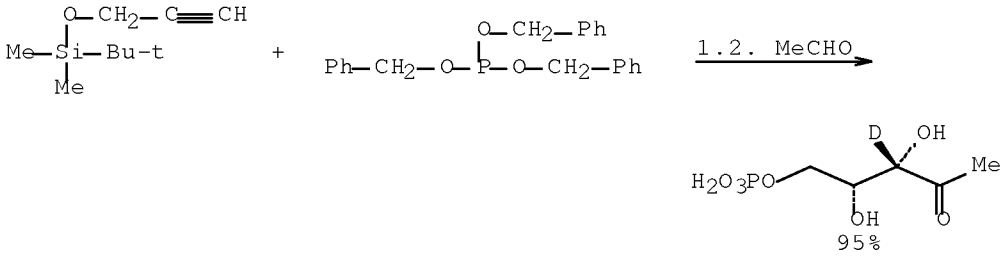
AB A method for synthesizing intermediates for use in the synthesis of carotenoid synthetic intermediates, carotenoid analogs, and/or carotenoid derivs. I [R1, R2 = Ra, Rb, Rc, Rd, Re, Rf; R3 = H, Me; R4 = H, OH, CH2OH, CH2OR5, OR5, wherein at least one R4 = OR5; R5 = alkyl, aryl, alkyl-N(R7)2, aryl-N(R7)2,alkyl-N+(R7)3, aryl-N+(R7)3, alkyl-CO2R7, aryl-CO2R7, alkyl-CO2-, aryl-CO2-, CO2R8, P(:O)(OR8)2, S(:O)(OR8)2, amino acid, peptide, carbohydrate,C(:O)(CH2)nCO2R9, nucleoside, co-antioxidant; R7 = H, alkyl, aryl; R8 = H, alkyl, aryl, CH2Ph, co-antioxidant; R9 = H, alkyl, aryl, P(:O)(OR8)2, S(:O)(OR8)2, amino acid, peptide, carbohydrate, nucleoside, co-antioxidant; n = 1 - 9]. Thus, lycophyll disuccinate disodium salt [II; R' = CH2CH:CHMeCH2OC(:O)(CH2)2CO2Na-(E)] was prepared from crocetindialdehyde via Wittig reaction with (E,E)-Br- Ph3P+CH2CH:CMeCH2CH2CH:CMeCO2Me in PhMe containing LiOH in MeOH, reduction with Dibal-H/PhMe in THF, diacylation with succinic anhydride in CH2Cl2 containing EtN(CHMe2)2, and sodium salt formation with NaOMe in MeOH. Methods for preparation of crocetindialdehyde and the phosphonium salt are also given. The carotenoid analog, derivative, or

intermediate may be administered to a subject for the inhibition and/or amelioration of any disease that involves production of reactive oxygen species, reactive nitrogen species, radicals and/or non-radicals. In some embodiments, the invention may include methods for synthesizing chemical compds. including an analog or derivative of a carotenoid. Carotenoid analogs or derivs. may include acyclic end groups. In some embodiments, a carotenoid analog or derivative may include at least one substituent. The substituent may enhance the solubility of the carotenoid analog or derivative such that the carotenoid analog or derivative at least partially dissolves in water.

RX(127) OF 304 - REACTION DIAGRAM NOT AVAILABLE

L3 ANSWER 2 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 147:316938 CASREACT Full-text
TITLE: The chemical mechanism of D-1-deoxyxylulose-5-phosphate reductoisomerase from Escherichia coli
AUTHOR(S): Wong, Ursula; Cox, Russell J.
CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS81TS, UK
SOURCE: Angewandte Chemie, International Edition (2007), 46(26), 4926-4929
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The 3-[2H]- and 4-[2H]-labeled 1-deoxyxylulose-5-phosphate were synthesized and used to investigate the chemical mechanism of D-1-deoxyxylulose-5-phosphate reductoisomerase (DXR) from E. coli. The observation of inverse secondary kinetic isotope effects for both labeled substrates indicates that DXR uses a retro-aldol/aldol mechanism in which the recombination reaction is the rate-limiting step.

RX(85) OF 110 - 7 STEPS

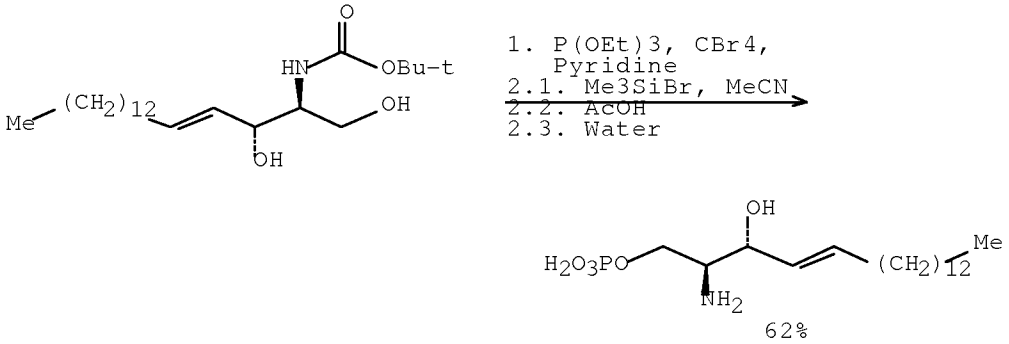


NOTE: 2) in-situ generated reagent (stage 1), regioselective, 4) regioselective, 5) Dess-Martin oxidation, 6) stereoselective
CON: STEP(1.1) room temperature -> -10 deg C; <0 deg C; 10 minutes, <0 deg C; 2 hours, room temperature; room temperature -> -40 deg C
STEP(1.2) 1 hour, -40 deg C
STEP(1.3) 20 minutes, room temperature
STEP(2.1) 30 minutes, reflux; reflux -> 0 deg C
STEP(2.2) 0 deg C; 1 hour, 0 deg C; 0 deg C -> room temperature
STEP(2.3) room temperature
STEP(3) 2 hours, room temperature
STEP(4.1) -20 deg C; 20 minutes, -20 deg C -> room temperature
STEP(4.2) 40 minutes, -30 deg C; 1 hour, -30 deg C -> room temperature
STEP(5.1) 2 hours, room temperature
STEP(5.2) 20 minutes, room temperature
STEP(6.1) room temperature; room temperature -> -20 deg C
STEP(6.2) -20 deg C; 3 hours, -20 deg C -> room temperature
STEP(6.3) overnight, room temperature, pH 2
STEP(7) 4.5 hours, room temperature, 1 atm

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 147:301368 CASREACT Full-text
TITLE: A Concise and Scalable Synthesis of High Enantiopurity (-)-D-erythro-Sphingosine Using Peptidyl Thiol Ester-Boronic Acid Cross-Coupling
AUTHOR(S): Yang, Hao; Liebeskind, Lanny S.
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (2007), 9(16), 2993-2995
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A short and efficient synthesis of high enantio-purity (-)-D-erythro-sphingosine has been achieved in 71% yield over 6 steps from N-Boc-L-serine. The key steps are high yield, racemization-free, palladium-catalyzed, copper(I)-mediated coupling of the thio-Ph ester of N-Boc-O-TBS-L-serine with E-1-pentadecenyl boronic acid and the highly diastereoselective reduction of the resulting peptidyl ketone with LiAl(O-t-Bu)3H. By using this concise route (-)-D-erythro-sphingosine can be prepared on large scale and in high enantio- and diastereo-purity (ee >99%, de up to 99%).

RX(60) OF 115 - 2 STEPS



62%

CON: STEP(1.1) 0 deg C; 30 minutes, 0 deg C;
0 deg C -> room temperature; 3 hours, room temperature
STEP(2.1) 2 hours, room temperature
STEP(2.2) heated
STEP(2.3) cooled

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:380213 CASREACT Full-text

TITLE: A convenient synthesis of 2-C-methyl-D-erythritol 4-phosphate and isotopomers of its precursor

AUTHOR(S): Koumbis, Alexandros E.; Kotoulas, Stefanos S.; Gallos, John K.

CORPORATE SOURCE: Laboratory of Organic Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 541 24, Greece

SOURCE: Tetrahedron (2007), 63(10), 2235-2243
CODEN: TETRAB; ISSN: 0040-4020

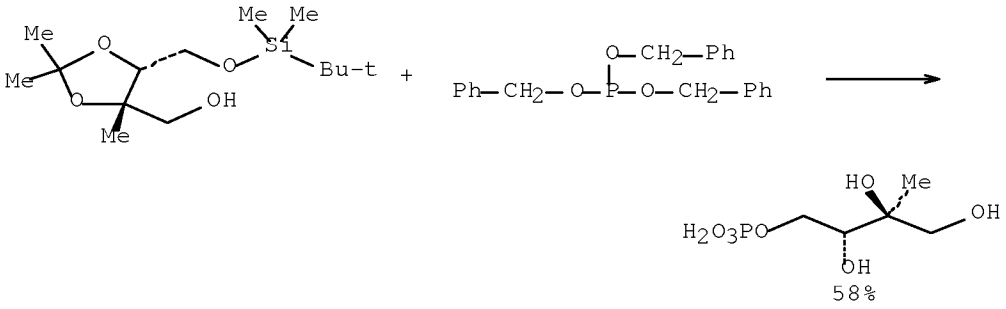
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new synthetic approach toward 2-C-methyl-D-erythritol 4-phosphate (MEP), a key intermediate in the mevalonate-independent biosynthetic pathway for isoprenoids, and deuterated analogs of its precursor, 2-C-methyl-D- erythritol acetonide, is described. This procedure uses 2-C-methyl-D-erythrose acetonide as starting material and delivers, through a mono-protection strategy, the target compds. in a short way and in high yield.

RX(166) OF 203 - 5 STEPS

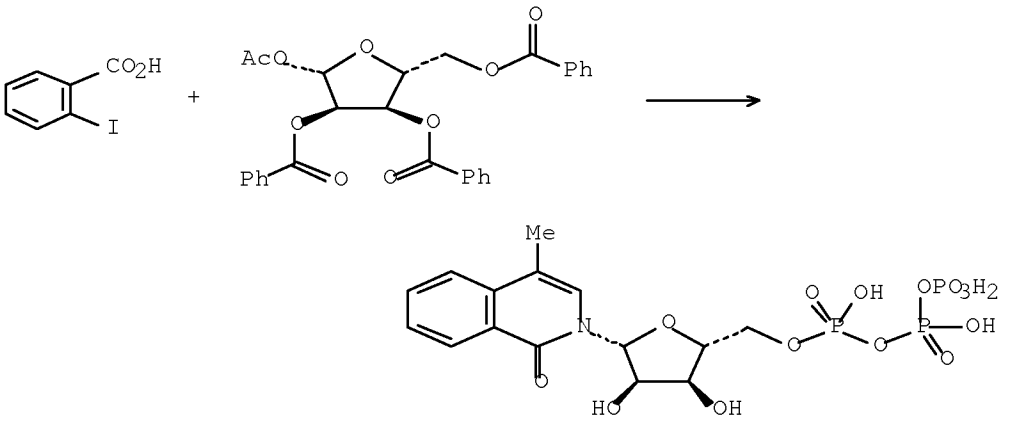


CON: STEP(1.1) 1 hour, room temperature
STEP(1.2) 24 hours, room temperature
STEP(2) 6 hours, room temperature
STEP(3.1) room temperature -> -10 deg C; 5 minutes, -10 deg C; 1 hour, -10 deg C -> room temperature; room temperature -> 0 deg C
STEP(3.2) 30 minutes, 0 deg C
STEP(4.1) room temperature -> -10 deg C; 15 minutes, -10 deg C; 3 hours, -10 deg C -> room temperature
STEP(4.2) room temperature, pH 6
STEP(5.1) 25 deg C
STEP(5.2) 60 deg C

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 146:317142 CASREACT Full-text
TITLE: Novel nucleotide triphosphates as potent P2Y2 agonists
AUTHOR(S): Brookings, Daniel; Davenport, Richard J.; Davis, Jeremy; Galvin, Frances C. A.; Lloyd, Steve; Mack, Stephen R.; Owens, Ray; Sabin, Verity; Wynn, Joanne
CORPORATE SOURCE: Granta Park, UCB-Group, Cambridge, CB1 6GS, UK
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(2), 562-565
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and P2Y2 activities of a novel series of nucleoside triphosphates are described. Many of these compds. were potent agonists of the P2Y2 receptor.

RX(42) OF 50 - 2 STEPS



NOTE: 2) analogues have similar reaction

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:100951 CASREACT Full-text

TITLE: Versatile Synthetic Method for Sphingolipids and Functionalized Sphingosine Derivatives via Olefin Cross Metathesis

AUTHOR(S): Yamamoto, Tetsuya; Hasegawa, Hiroko; Hakogi, Toshikazu; Katsumura, Shigeo

CORPORATE SOURCE: School of Science and Technology, Kwansei Gakuin University, 2-1 Gakuen, Sanda, Hyogo, 669-1337, Japan

SOURCE: Organic Letters (2006), 8(24), 5569-5572
CODEN: ORLEF7; ISSN: 1523-7060

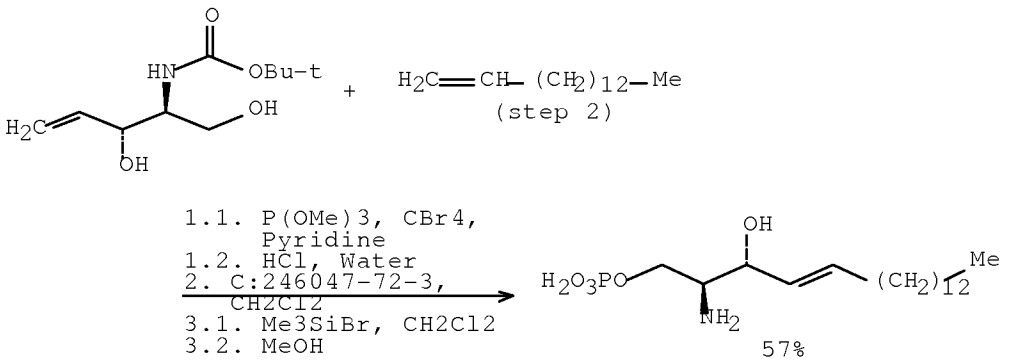
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A highly efficient and versatile method for the synthesis of various sphingolipids, such as sphingomyelin, ceramide, sphingosine, sphingosine 1-phosphate, and functionalized sphingosine derivs., was established by two types of combinations of the olefin cross metathesis reaction. One reaction was between the same olefin part and appropriate amino alcs., which were prepared starting from N-Boc-L-serine, and the other was between appropriate olefins and the same amino alc.

RX(74) OF 103 - 3 STEPS



NOTE: 1) molecular sieves used, 2) stereoselective
CON: STEP(1.1) -15 deg C; -15 deg C -> room temperature
STEP(1.2) 1 deg C
STEP(2.1) room temperature; 2 hours, reflux
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 10 minutes, room temperature

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:489429 CASREACT Full-text
TITLE: Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates
INVENTOR(S): Lockwood, Samuel F.; Nadolski, Geoff; Burdick, David; Tang, Peng Cho; Jackson, Henry L.; Fang, Zhiqiang; Du, Yishu; Yang, Min; Geiss, William; Williams, Richard
PATENT ASSIGNEE(S): Hawaii Biotech, Inc., USA
SOURCE: PCT Int. Appl., 59pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006119125	A2	20061109	WO 2006-US16487	20060501
WO 2006119125	A3	20070111		
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 20060293545	A1	20061228	US 2006-415375	20060501
EP 1879902	A2	20080123	EP 2006-751932	20060501
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IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
PRIORITY APPLN. INFO.: US 2005-675957P 20050429
US 2005-691518P 20050617
US 2005-692682P 20050621
US 2005-699653P 20050715
US 2005-702380P 20050726
US 2005-712350P 20050830
WO 2006-US16487 20060501
OTHER SOURCE(S): MARPAT 145:489429
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A method for synthesizing intermediates for use in the synthesis of carotenoid synthetic intermediates, carotenoid analogs, and/or carotenoid derivs. I [R1, R2 = Ra, Rb, Rc, Rn, Rm; R3 = H, Me; R4 = H, OH, CH2OH, OR5 with the proviso that at least one R4 = OR5; R5 = alkyl, aryl, alkyl-N(R7)2, aryl-N(R7)2, alkyl-N+(R7)3, aryl-N+(R7)3, alkyl-CO2R7, aryl-CO2R7, alkyl-CO2-, aryl-CO2-, CO2R8, P(:O)(OR8)2, S(:O)(OR8)2, amino acid, peptide, carbohydrate, C(:O)(CH2)nCO2R9, nucleoside, co-antioxidant; R7 = H, alkyl, aryl; R8 = H, alkyl, aryl, CH2Ph, co-antioxidant; R9 = H, alkyl, aryl, P(:O)(OR8)2, S(:O)(OR8)2, amino acid, peptide, carbohydrate, nucleoside, co-antioxidant; n = 1 - 9]. The carotenoid analog, derivative, or intermediate may be administered to a subject for the inhibition and/or amelioration of any disease that involves production of reactive oxygen species, reactive nitrogen species, radicals and/or non-radicals. In some embodiments, the invention may include methods for synthesizing chemical compds. including an analog or derivative of a carotenoid. Carotenoid analogs or derivs. may include acyclic end groups. In some embodiments, a carotenoid analog or derivative may include at least one substituent. The substituent may enhance the solubility of the carotenoid analog or derivative such that the carotenoid analog or derivative at least partially dissolves in water. Thus, lycophyll disuccinate (II) was prepared from acetic acid 3,7-dimethyl-8-oxo-2,6-octadienyl ester via allylic oxidation with NaClO2 in Me3COH containing 2-methyl-2-butene and NaH2PO3, deacetylation with K2CO3 in MeOH, esterification with MeI in aqueous MeOH containing K2CO3, bromination with CBr4 in THF containing PPh3, phosphinylation with PPh3 in EtOAc, Wittig reaction with crocetindialdehyde, all-E-OHC(CMe:CHCH:CH)2CH:CMeCH:CHCH:CMe CHO, in MeOH containing LiOH, reduction with Dibal-H in THF, and acylation with succinic anhydride in CH2Cl2 containing EtN(CHMe2)2.

RX(78) OF 156 - REACTION DIAGRAM NOT AVAILABLE

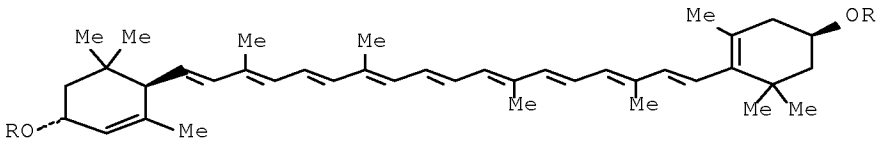
L3 ANSWER 8 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:377488 CASREACT Full-text
TITLE: Water-dispersible carotenoids, including analogs and derivatives
INVENTOR(S): Lockwood, Samuel F.; Nadolski, Geoff
PATENT ASSIGNEE(S): Hawaii Biotech, Inc., USA
SOURCE: PCT Int. Appl., 77pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006102576	A1	20060928	WO 2006-US10726	20060323
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
CA 2611137	A1	20060928	CA 2006-2611137	20060323
US 20070015735	A1	20070118	US 2006-388237	20060323
EP 1877372	A1	20080116	EP 2006-748636	20060323
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: US 2005-664478P 20050323
WO 2006-US10726 20060323

OTHER SOURCE(S): MARPAT 145:377488

GI



I

AB Carotenoid analogs or derivs., such as I [R is independently: alkyl; aryl; -alkyl-N(R7)2; -aryl-N(R7)2; -alkyl-N+ (R7)3; -aryl-N+(R7)3; -alkyl-CO2R7; -aryl-CO2R7; -alkyl-CO2; -aryl-CO2; -CO2R8; -P(O)(OR8)2; -S(O)(OR8)2; an amino acid; a peptide, a carbohydrate; -C(O)- (CH2)0-CO2R9; a nucleoside residue, or a co-antioxidant; wherein R7 is hydrogen, alkyl, or aryl; wherein R8 is hydrogen, alkyl, aryl, benzyl or a co-antioxidant; wherein R9 is hydrogen; alkyl; aryl; -P(O)(OR8)2; -S(O)(OR8)2; an amino acid; a peptide, a carbohydrate; a nucleoside, or a co-antioxidant], were prepared for therapeutic use in the inhibition and amelioration of diseases resulting in change and/or loss of vision. Thus, lutein disuccinate disodium salt I [R = CO(CH2)2CO2Na] was prepared starting from lutein I (R = H) and succinic anhydride and was evaluated for solubility and antioxidant properties.

RX(9) OF 14 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:137320 CASREACT Full-text
TITLE: Cell permeation of a Trypanosoma brucei aldolase inhibitor: Evaluation of different enzyme-labile phosphate protecting groups

AUTHOR(S): Azema, Laurent; Lherbet, Christian; Baudoin, Cecile; Blonski, Casimir

CORPORATE SOURCE: Laboratoire SPCMIB, Groupe de Chimie Organique Biologique, Universite Paul Sabatier UMR CNRS 5068, Toulouse, 31062, Fr.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(13), 3440-3443
CODEN: BMCLE8; ISSN: 0960-894X

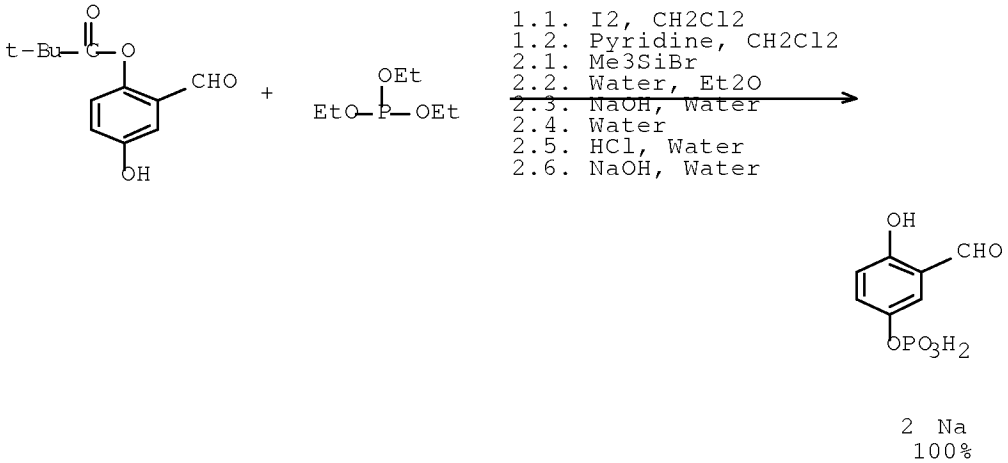
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of four prodrugs directed against Trypanosoma brucei aldolase bearing various transient enzyme-labile phosphate protecting groups was developed. Herein, we describe the synthesis and evaluation of cell permeation of these prodrugs. The oxymethyl derivative was the most efficient prodrug with a good recovering of the free drug (IC50 = 20 μM) and without any measurable cytotoxicity.

RX(14) OF 42 - 2 STEPS



CON: STEP(1.1) 0 deg C; 0 deg C -> room temperature
STEP(1.2) 30 minutes, 0 deg C
STEP(2.1) room temperature
STEP(2.2) 5 minutes, room temperature
STEP(2.3) room temperature, neutralized
STEP(2.4) overnight, room temperature
STEP(2.5) room temperature, pH 3
STEP(2.6) room temperature, neutralized

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:83603 CASREACT Full-text

TITLE: Synthesis and evaluation of a mechanism-based

inhibitor of a 3-deoxy-D-arabino heptulosonate 7-phosphate synthase

AUTHOR(S): Walker, Scott R.; Parker, Emily J.

CORPORATE SOURCE: Institute of Fundamental Sciences, Massey University, Palmerston North, N. Z.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(11), 2951-2954
CODEN: BMCLE8; ISSN: 0960-894X

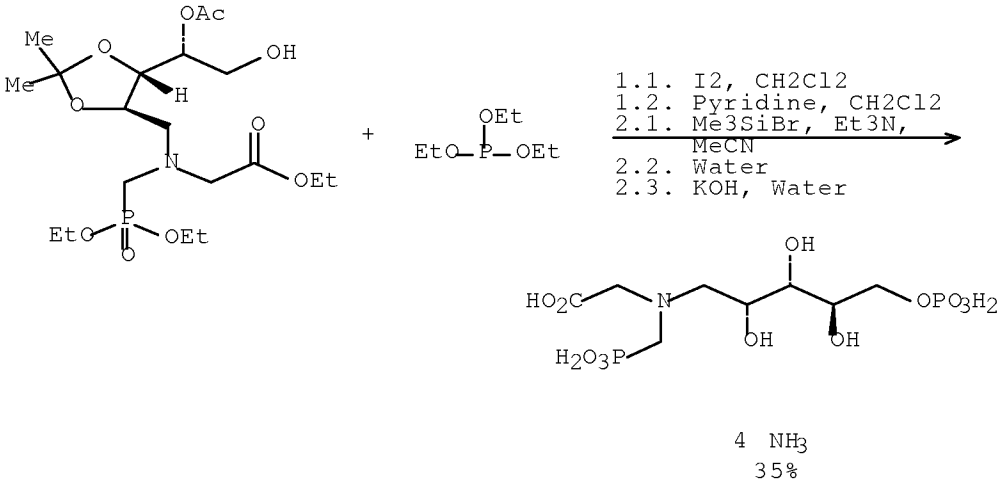
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The first mechanism-based inhibitor of a 3-deoxy-D-arabino heptulosonate 7-phosphate (DAH7P) synthase has been synthesized in 12 steps from D-arabinose, and has been found to be a very slow binding inhibitor of Escherichia coli DAH7P synthase.

RX(17) OF 45 - 2 STEPS



CON: STEP(2.1) 4 deg C
STEP(2.2) 75 deg C
STEP(2.3) 75 deg C

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 144:365182 CASREACT Full-text

TITLE: Selective Irreversible Inhibition of Fructose 1,6-Bisphosphate Aldolase from Trypanosoma brucei

AUTHOR(S): Dax, Chantal; Duffieux, Francis; Chabot, Nicolas; Coincon, Mathieu; Sygusch, Jurgen; Michels, Paul A. M.; Blonski, Casimir

CORPORATE SOURCE: Groupe de Chimie Organique Biologique, LSPCMIB, UMR-CNRS 5068, Universite Paul Sabatier, Toulouse, 31062, Fr.

SOURCE: Journal of Medicinal Chemistry (2006), 49(5), 1499-1502
CODEN: JMCMAR; ISSN: 0022-2623

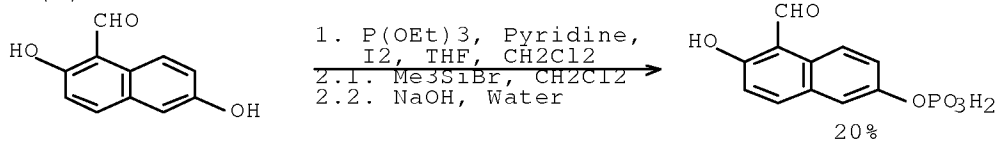
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An irreversible competitive inhibitor hydroxynaphthaldehyde phosphate was synthesized that is highly selective against the glycolytic enzyme fructose 1,6-bisphosphate aldolase from Trypanosoma brucei (causative agent of sleeping sickness). Inhibition involves Schiff base formation by the inhibitor aldehyde with Lys116 followed by reaction of the resultant Schiff base with a second residue. Mol. simulations indicate significantly greater mol. geometries conducive for nucleophilic attack in T. brucei aldolase than the mammalian isoenzyme and suggest Ser48 as the Schiff base modifying residue.

RX(7) OF 10 - 2 STEPS



20%

NOTE: 1) regioselective
CON: STEP(1.1) 30 minutes, 0 deg C; overnight, room temperature
STEP(2.1) 3 hours, room temperature
STEP(2.2) room temperature, pH 7.2

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 144:331573 CASREACT Full-text

TITLE: Total Synthesis of Geranylgeranylglyceryl Phosphate Enantiomers: Substrates for Characterization of 2,3-O-Digeranylgeranylglyceryl Phosphate Synthase

AUTHOR(S): Zhang, Honglu; Shibuya, Kyohei; Hemmi, Hisashi; Nishino, Tokuzo; Prestwich, Glenn D.

CORPORATE SOURCE: Department of Medicinal Chemistry, The University of Utah, Salt Lake City, UT, 84108-1257, USA

SOURCE: Organic Letters (2006), 8(5), 943-946
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

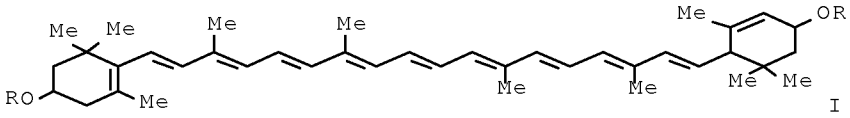
LANGUAGE: English

AB To det. the enantioselectivity of (S)-2,3-di-O-geranylgeranylglyceryl phosphate synthase (DGGGPS) from the thermoacidophilic archaeon Sulfolobus solfataricus, we developed an efficient enantioselective route to the enantiomeric geranylgeranylglyceryl phosphates (R)-GGGP and (S)-GGGP. Previous routes to these substrates involved enzymic conversions due to the lability of the polyprenyl chains toward common phosphorylation reaction conditions. The synthesis described herein employs a mild tri-Me phosphite/carbon tetrabromide oxidative phosphorylation to circumvent this problem. In contrast to previous results suggesting that only (S)-GGGP can act as the prenyl acceptor substrate, both (R)-GGGP and (S)-GGGP were found to be substrates for DGGGPS.

RX(16) OF 33 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 144:274430 CASREACT Full-text
TITLE: The synthesis and aqueous superoxide anion scavenging of water-dispersible lutein esters
AUTHOR(S): Nadolski, Geoff; Cardounel, Arturo J.; Zweier, Jay L.; Lockwood, Samuel F.
CORPORATE SOURCE: Hawaii Biotech, Inc., Aiea, HI, 96701, USA
SOURCE: Bioorg. Med. Chem. Lett. (2006), 16(4), 775-781
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Xanthophyll carotenoids of the C40 series, which includes com. important compds. such as lutein, zeaxanthin, and astaxanthin, have poor aqueous solubility in the native state. Hawaii Biotech, Inc. (HBI) and others have shown that the aqueous dispersibility of derivatized carotenoids can be increased by varying the chemical structure of the esterified moieties. In the current study, the published series of novel, highly water-dispersible C40 carotenoid derivs. has been extended to include derivs. of (3R,3'R,6'R)-lutein [β,ε-carotene-3,3'-diol (I; R = H)]. Two novel derivs. were synthesized by esterification with inorg. phosphate and succinic acid, resp., and subsequently converted to the sodium salts. Red-orange, clear, aqueous suspensions were obtained after addition of these novel derivs. to USP-purified water. Aqueous dispersibility of lutein disuccinate sodium salt (I; R = COCH2CH2CO2Na) was 2.85 mg/mL; the diphosphate salt I [R = P:O(ONa)2] demonstrated a >10-fold increase in dispersibility at 29.27 mg/mL. As reported previously, these aqueous suspensions were obtained without the addition of heat, detergents, co-solvents, or other additives. The direct aqueous superoxide scavenging abilities of these novel derivs. were subsequently evaluated by ESR (EPR) spectroscopy in a well-characterized in vitro isolated human neutrophil assay. The novel derivs. were nearly identical aqueous-phase scavengers, demonstrating dose-dependent suppression of the superoxide anion signal (as detected by spin-trap adducts of DEPMPO) in the millimolar range. These lutein-based soft drugs will likely find utility in those com. and clin. applications for which aqueous-phase singlet oxygen quenching and direct radical scavenging may be required.

RX(7) OF 8 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 144:254122 CASREACT Full-text
TITLE: Preparation of indazole derivatives and ophthalmic

compositions for treating ocular hypertension

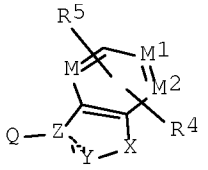
INVENTOR(S): Doherty, James B.; Shen, Dong-Ming
PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

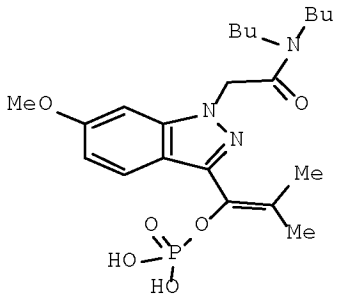
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006020003	A2	20060223	WO 2005-US25136	20050715
WO 2006020003	A3	20060831		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005274972	A1	20060223	AU 2005-274972	20050715
CA 2574078	A1	20060223	CA 2005-2574078	20050715
EP 1771170	A2	20070411	EP 2005-771451	20050715
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1988903	A	20070627	CN 2005-80024510	20050715
JP 2008507521	T	20080313	JP 2007-522582	20050715
US 20080032951	A1	20080207	US 2006-630172	20061219
IN 2006CN04793	A	20071005	IN 2006-CN4793	20061229
PRIORITY APPLN. INFO.:			US 2004-589444P	20040720
			WO 2005-US25136	20050715

OTHER SOURCE(S): MARPAT 144:254122

GI



I

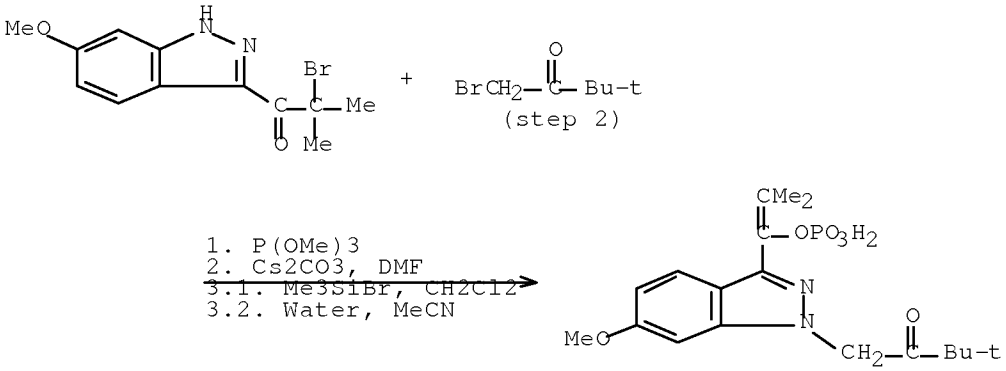


II

AB Title compds. I [M, M1, M2 = CH or N; Z = N or C, when Z = N then the bond between Y and Z is a single bond and between X and Y resp. represents CR1=N, CR1=CR1a, CR1a=CR1, or N=CR1, and when Z = C then X = O or S, Y represents CR1 and the bond between Y and Z is a double bond; R4 and R5 independently = H,

OH, alkoxy, etc.; Q = unsatd. phosphonate derivative or substituted carbonyl alkyl derivative; R1 = OH, alkoxy,, unsatd. phosphonate derivative, etc.; R1a = H, (un)substituted alkyl, cycloalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as potassium channel blockers suitable for ophthalmic compns. fore treatment of glaucoma and other conditions which leads to elevated intraoccular pressure in the eye of a patient. Thus, e.g., II was prepared by amidation of (3-isobutyryl-6-methoxy-1H-indazol-1-yl)acetic acid (preparation given) with di-n-butylamine. In assays for evaluating ability to block potassium channels, I was determined to possess IC50's in the range of about 1nM to about 20 μM. This invention also relates to the use of such compds. to provide a neuroprotective effect to the eye of mammalian species, particularly humans.

RX(123) OF 346 - 3 STEPS

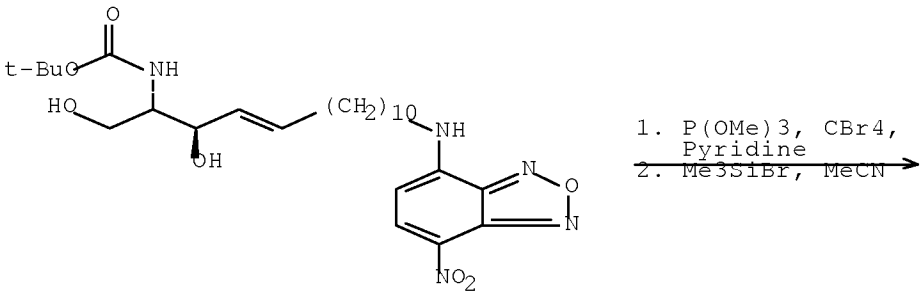


NOTE: 1) Perkow reaction, 2) regioselective
CON: STEP(1) 21 hours, 62 deg C
STEP(2.1) 2 hours, room temperature; 1 day, 50 deg C
STEP(3.1) cooled; 2.5 hours, room temperature

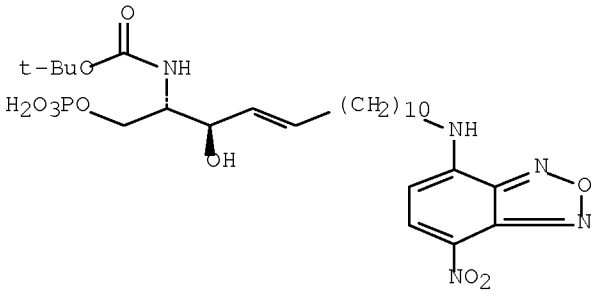
L3 ANSWER 15 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 144:121266 CASREACT Full-text
TITLE: NBD-labeled derivatives of the immunomodulatory drug FTY720 as tools for metabolism and mode of action studies
AUTHOR(S): Ettmayer, Peter; Baumruker, Thomas; Guerini, Danilo; Mechtcheriakova, Diana; Nussbaumer, Peter; Streiff, Markus B.; Billich, Andreas
CORPORATE SOURCE: Novartis Institutes for BioMedical Research, Vienna, A-1230, Austria
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(1), 84-87
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Fluorescently labeled chiral analogs of the immunomodulatory drug FTY720 and its corresponding phosphates with variable aliphatic spacers between the aromatic ring and the NBD label have been synthesized. Determining the influence of the spacer on the in vitro phosphorylation rate by SPHK1 and 2

resulted in the identification of NBD-(R)-AAL 1c,d which are phosphorylated with an efficiency comparable to that of the unlabeled FTY720 analog (R)-AAL. Furthermore, the NBD-(R)-AAL phosphates 10c,d were proven to be a functional S1P receptor agonist.

RX(37) OF 65 - 2 STEPS



RX(37) OF 65 - 2 STEPS



56%

CON: STEP(1) -10 deg C -> room temperature
STEP(2) room temperature

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 143:229650 CASREACT Full-text
TITLE: Photoaffinity-labeled sphingomyelin analogs and processes thereof
INVENTOR(S): Katsumura, Shigeo; Hakogi, Toshikazu; Shigenari, Toshihiko
PATENT ASSIGNEE(S): Daiso Co., Ltd., Japan
SOURCE: U.S. Pat. Appl. Publ., 15 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

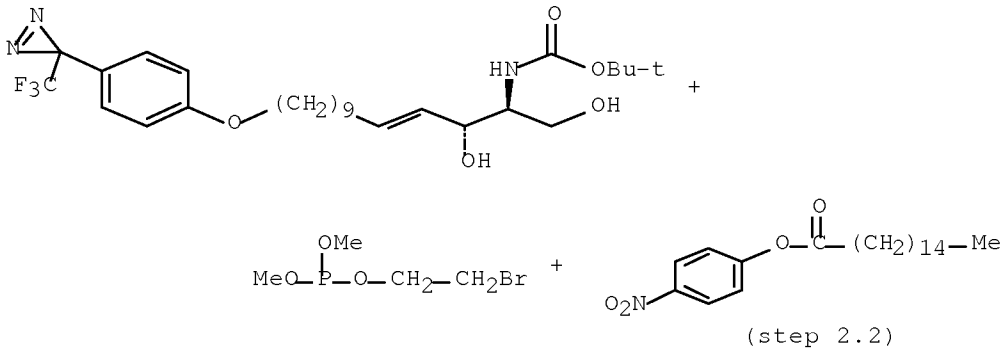
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050182265	A1	20050818	US 2004-934571	20040907
US 7084285	B2	20060801		
JP 2005263774	A	20050929	JP 2004-264995	20040913

PRIORITY APPLN. INFO.: JP 2004-41750 20040218
OTHER SOURCE(S): MARPAT 143:229650
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

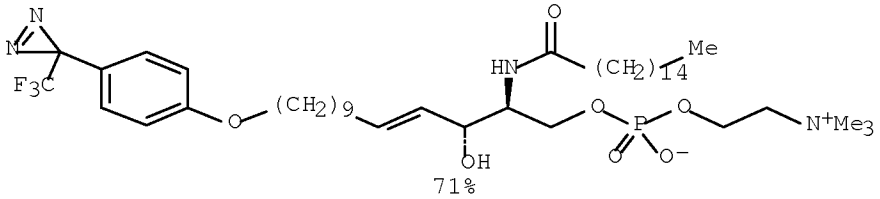
AB A photoaffinity-labeled sphingomyelin analogs s I (Y1, Y2 are different from each other and are R5 or ZOR1; R5 = C1-20 alkyl, aryl group or C1-6 alkyl group substituted by aryl group, Z is a photoaffinity-labeled group; R1 = C1-20 alkylene) or an optically active compound thereof were prepared Thus, the TFDP-sphingomyelin II was prepared in a multistep procedure starting from the triol III. The TFDP-sphingomyelin IV was similarly prepared

RX(30) OF 53 - 3 STEPS



(step 2.2)

RX(30) OF 53 - 3 STEPS
1.1. CBr4, Pyridine
1.2. HCl, Water
2.1. F3CCO2H, CH2Cl2
2.2. Et3N, THF
3. Me3N, MeOH



71%

CON: STEP(1.1) 0 deg C; 3.5 hours, 0 deg C;
0 deg C -> room temperature
STEP(1.2) room temperature, neutralized
STEP(2.1) 0 deg C; 5 hours, 0 deg C
STEP(2.2) 0 deg C; 1 day, room temperature
STEP(3.1) room temperature; 1 day, room temperature

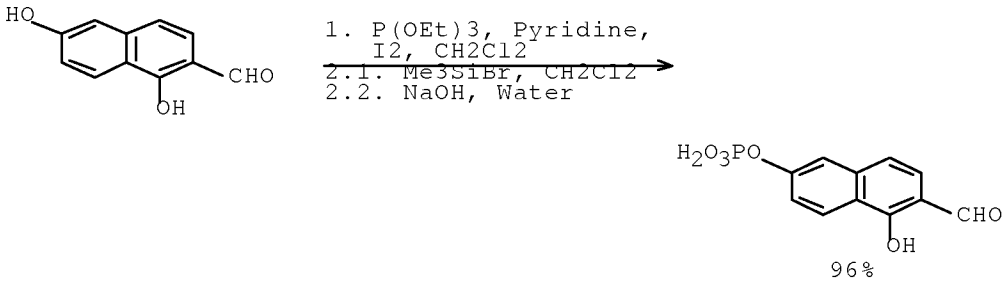
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:458992 CASREACT Full-text
TITLE: Hydroxynaphthaldehyde Phosphate Derivatives as Potent Covalent Schiff Base Inhibitors of Fructose-1,6-bisphosphate Aldolase
AUTHOR(S): Dax, Chantal; Coincon, Mathieu; Sygusch, Jurgen; Blonski, Casimir
CORPORATE SOURCE: Groupe de Chimie Organique Biologique, LSPCMIB UMR CNRS 5068, Universite Paul Sabatier, Toulouse, 31062, Fr.
SOURCE: Biochemistry (2005), 44(14), 5430-5443
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Interactions of phosphate derivs. of 2,6-dihydroxynaphthalene (NA-P2) and 1,6-dihydroxy-2-naphthaldehyde (HNA-P, phosphate at position 6) with fructose-1,6-bisphosphate aldolase from rabbit muscle were analyzed by enzyme kinetics, difference spectroscopy, site-directed mutagenesis, mass spectrometry, and mol. dynamics. Enzyme activity was competitively inhibited by NA-P2, whereas HNA-P exhibited slow-binding inhibition with an overall inhibition constant of .apprx.24 nM. HNA-P inactivation was very slowly reversed with t1/2 .apprx.10 days. Mass spectrometry and spectrophotometric absorption indicated that HNA-P inactivation occurs by Schiff base formation. Rates of enzyme inactivation and Schiff base formation by HNA-P were identical and corresponded to .apprx.4 HNA-P mols. bound par aldolase tetramer at maximal inhibition. Site-directed mutagenesis of conserved active site lysine residues 107, 146, and 229 and Asp-33 indicated that Schiff base formation by HNA-P involved Lys-107 and was promoted by Lys-146. Titration of Lys-107 by pyridoxal 5-phosphate yielded a microscopic pKa .apprx.8 for Lys-107, corroborating a role as nucleophile at pH 7.6. Site-directed mutagenesis of Ser-271, an active site residue that binds the C1-phosphate of dihydroxyacetone phosphate, diminished HNA-P binding and enabled modeling of HNA-P in the active site. Mol. dynamics showed persistent HNA-P phosphate interactions with the C1-phosphate binding site in the noncovalent adduct. The naphthaldehyde hydroxyl, ortho to the HNA-P aldehyde, was essential for promoting carbinolamine precursor formation by

intramol. catalysis. The simulations indicate a slow rate of enzyme inactivation due to competitive inhibition by the phenate form of HNA-P, infrequent nucleophilic attack in the phenol form, and significant conformational barrier to bond formation as well as electrostatic destabilization of protonated ketimine intermediates. Solvent accessibility by Lys-107 Nz was reduced in the covalent Schiff base complex, and in those instances where water mols. interacted with Lys-107 in the simulations, Schiff base hydrolysis was not mechanistically favorable. The findings at the mol. level corroborate the observed mechanism of slow-binding tight inhibition by HNA-P of muscle aldolase and should serve as a blueprint for future aldolase inhibitor design.

RX(9) OF 15 - 2 STEPS



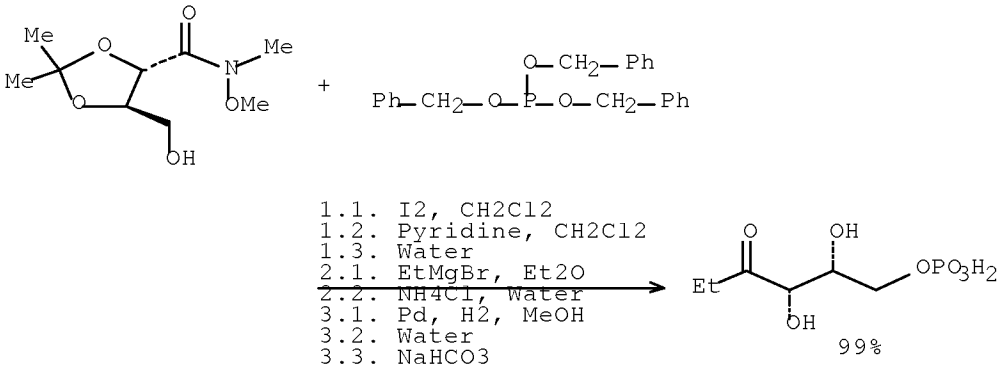
CON: STEP(1.1) 1 hour, 0 deg C; 0 deg C -> room temperature
STEP(2.1) room temperature; 3 hours, room temperature
STEP(2.2) room temperature, pH 7.6

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:392567 CASREACT Full-text
TITLE: Synthesis and Evaluation of 1-Deoxy-D-xylulose 5-Phosphoric Acid Analogues as Alternate Substrates for Methylerythritol Phosphate Synthase
AUTHOR(S): Fox, David T.; Poulter, C. Dale
CORPORATE SOURCE: Department of Chemistry, University of Utah, Salt Lake City, UT, 84112, USA
SOURCE: Journal of Organic Chemistry (2005), 70(6), 1978-1985
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Four deoxyxylulose phosphate (DXP) analogs were synthesized and evaluated as substrates/inhibitors for methylerythritol phosphate (MEP) synthase. In analogs CF3-DXP (I), CF2-DXP (II), and CF-DXP (III), the three Me hydrogens at C1 of DXP were sequentially replaced by fluorine. In the fourth analog, Et-DXP (IV), the Me group in DXP was replaced by an Et moiety. Analogs I, II, and IV were not substrates for MEP synthase under normal catalytic conditions and were instead modest inhibitors with IC50 values of 2.0, 3.4, and 6.2 mM, resp. In contrast, III was a good substrate (kcat = 38 s-1, Km = 227 μM) with a turnover rate similar to that of the natural substrate. These results are consistent with a retro-aldol/aldol mechanism rather than an α-ketol rearrangement for the enzyme-catalyzed conversion of DXP to MEP.

RX(66) OF 78 - 3 STEPS



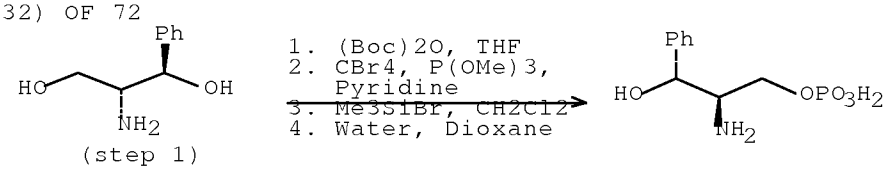
CON: STEP(1.1) -40 deg C
STEP(1.2) 10 minutes, -40 deg C; 1 hour, -40 deg C -> room temperature
STEP(1.3) room temperature
STEP(2.1) -40 deg C; 1 hour, -40 deg C
STEP(2.2) -40 deg C
STEP(3.1) 6 hours, room temperature
STEP(3.2) 2 days, room temperature
STEP(3.3) room temperature, pH 7

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:374041 CASREACT Full-text
TITLE: Synthesis and biological properties of novel sphingosine derivatives
AUTHOR(S): Murakami, Teiichi; Furusawa, Kiyotaka; Tamai, Tadakazu; Yoshikai, Kazuyoshi; Nishikawa, Masazumi
CORPORATE SOURCE: National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8565, Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(4), 1115-1119
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sphingosine-1-phosphate (S-1P) derivs. such as threo-(2S,3S)-analogs, which are C-3 stereoisomers of natural erythro-(2S,3R)-S-1P, have been synthesized starting from -serine or (1S,2S)-2-amino-1-aryl-1,3- propanediols. Threo-(1S,2R)-2-amino-1-aryl-3-bromopropanols (HBr salt) have also been prepared from (1S,2S)-2-amino-1-aryl-1,3-propanediols. The threo-S-1Ps and the threo-amino-bromide derivs. have shown potent inhibitory activity against Ca2+ ion mobilization in HL60 cells induced by erythro-S-1P, suggesting that these compds. would compete with cell surface EDG/S1P receptors.

RX(32) OF 72



(step 1)

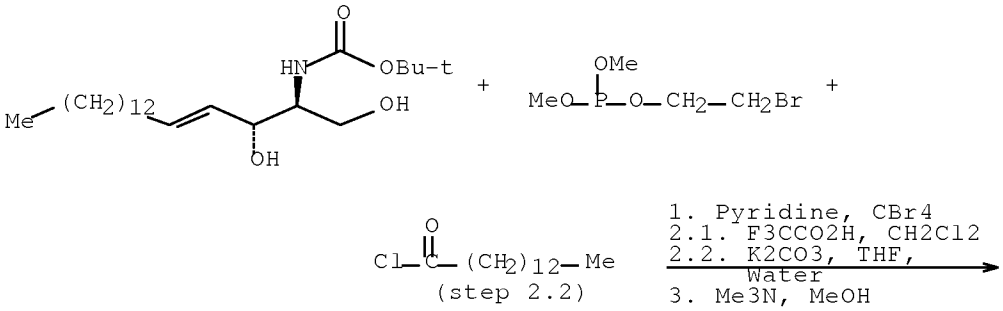
NOTE: regioselective stage 2
CON: STAGE(2) 5 deg C -> room temperature
STAGE(3) 3 hours, room temperature

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:197743 CASREACT Full-text
TITLE: Cross metathesis route in sphingomyelin synthesis
AUTHOR(S): Hasegawa, Hiroko; Yamamoto, Tetsuya; Hatano, Sho; Hakogi, Toshikazu; Katsumura, Shigeo
CORPORATE SOURCE: School of Science and Technology, Kwansei Gakuin University, Hyogo, 669-1337, Japan
SOURCE: Chemistry Letters (2004), 33(12), 1592-1593
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

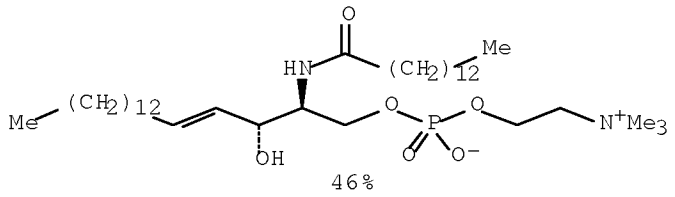
AB Cross metathesis reaction of short chain Boc sphingosine using Grubbs' 2nd generation catalyst proceeded in stereoselective manner to afford Boc sphingosine in good yield. An efficient synthesis of sphingomyelin was achieved from the obtained Boc sphingosine using the phosphorylation reagent (MeO)2POCH2CH2Br.

RX(19) OF 21 - 3 STEPS



(step 2.2)

RX(19) OF 21 - 3 STEPS



46%

CON: STEP(1) 0 deg C
STEP(2) 0 deg C

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:177000 CASREACT Full-text
TITLE: A short, concise route to diphosphatidylglycerol (cardiolipin) and its variants
AUTHOR(S): Krishna, U. Murali; Ahmad, Moghis U.; Ali, Shoukath M.; Ahmad, Imran
CORPORATE SOURCE: NeoPharm, Inc., Waukegan, IL, 60085, USA
SOURCE: Lipids (2004), 39(6), 595-600
CODEN: LPDSAP; ISSN: 0024-4201
PUBLISHER: AOCS Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new approach is described for the synthesis of the cardiolipin family of phospholipids that uses phosphonium salt methodol. The method involves the reaction of 2-O-protected glycerol with a trialkyl phosphite derived from 1,2-diacyl-sn-glycerol in the presence of pyridinium bromide perbromide and triethylamine to afford the phosphoric triesters. The synthesis involves three steps and allows the preparation of a wide range of cardiolipins with different substitution patterns and chain lengths, including unsatd. derivs. The use of inexpensive protecting groups and the ease of purification facilitate this synthetic route and allow its scale-up in a higher overall yield (72%) than the literature methods.

RX(11) OF 31 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

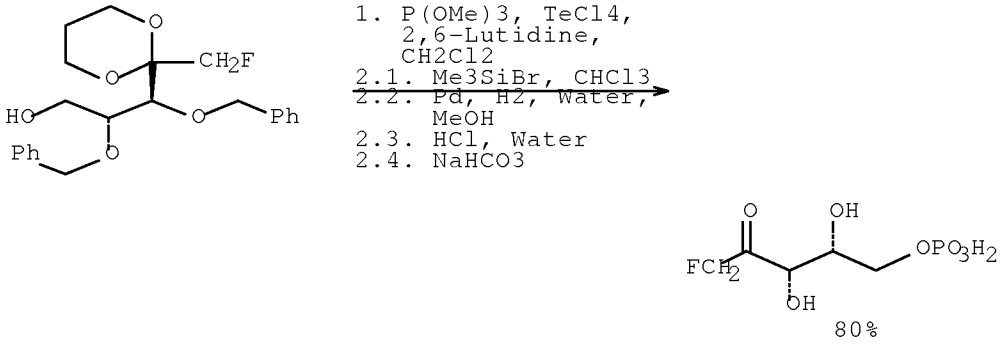
L3 ANSWER 22 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 141:424374 CASREACT Full-text
TITLE: Chemical synthesis of the second messenger nicotinic acid and adenine dinucleoside phosphate by total synthesis of nicotinamide adenine dinucleotide phosphate
AUTHOR(S): Dowden, James; Moreau, Christelle; Brown, Richard S.; Berridge, Georgina; Galione, Antony; Potter, Barry V. L.
CORPORATE SOURCE: Wolfson Laboratory of Medical Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Bath, BA2 7AY, UK
SOURCE: Angewandte Chemie, International Edition (2004), 43(35), 4637-4640

CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The first single-isomer synthesis of NADP is reported. Installation and maintenance of sensitive phosphate and pyridinium functionalities were key to success. Significantly, conversion of NADP into the important mammalian second messenger nicotinic acid adenine dinucleotide phosphate (NAADP) was achieved. The biol. evaluation of the activity of the release of Ca2+ ions confirms the identity of NAADP. Ca2+ release properties against sea-urchin-egg homogenate and spectroscopic characterization are reported.

RX(21) OF 44 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 141:390902 CASREACT Full-text
TITLE: Study of 1-Deoxy-D-xylulose-5-phosphate Reductoisomerase: Synthesis and Evaluation of Fluorinated Substrate Analogues
AUTHOR(S): Wong, Alexander; Munos, Jeffrey W.; Devasthali, Vidusha; Johnson, Kenneth A.; Liu, Hung-wen
CORPORATE SOURCE: Division of Medicinal Chemistry, College of Pharmacy and Department of Chemistry and Biochemistry, University of Texas, Austin, TX, 78712, USA
SOURCE: Organic Letters (2004), 6(20), 3625-3628
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1-Deoxy-D-xylulose-5-phosphate (DXP) reductoisomerase is a NADPH-dependent enzyme catalyzing the conversion of DXP to methyl-D-erythritol 4-phosphate (MEP). In this study, each of the hydroxyl groups in DXP and one of its C-1 hydrogen atoms, were sep. replaced with a fluorine atom and the effect of the substitution on the catalytic turnover was examined The 1-fluoro-DXP is a poor substrate, while both 3- and 4-fluoro-DXP behave as noncompetitive inhibitors.

RX(44) OF 237 - 2 STEPS



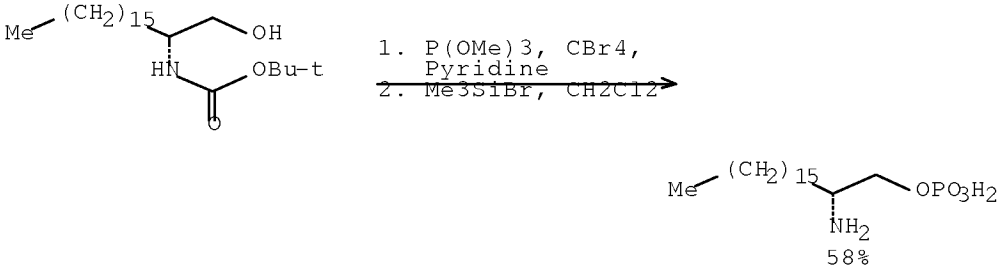
CON: STEP(1) 1.5 hours, room temperature
STEP(2.1) 1.5 hours, room temperature
STEP(2.2) 17 hours, room temperature
STEP(2.3) 12 hours, 37 deg C
STEP(2.4) room temperature, neutralized

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 141:54546 CASREACT Full-text
TITLE: Syntheses of sphingosine-1-phosphate analogues and their interaction with EDG/S1P receptors
AUTHOR(S): Lim, Hyun-Suk; Park, Jeong-Ju; Ko, Kwangseok; Lee, Mee-Hyun; Chung, Sung-Kee
CORPORATE SOURCE: Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2499-2503
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sphingosine-1-phosphate (S1P) is an important regulator of a wide variety of biol. processes acting as an endogenous ligand to EDG/S1P receptors. In an effort to establish structure-activity relationship between EDG/S1P and ligands, the authors report herein homol. modeling study of EDG-1/S1P1, syntheses of S1P analogs, and cell based binding affinity study for EDG/S1P receptors.

RX(88) OF 285 - 2 STEPS



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:321601 CASREACT Full-text

TITLE: Chemical resolution of 1,2-O-cyclohexylidene-3,4-O-(tetraisopropyldisiloxane-1,3-diyl)-myo-inositol and synthesis of phosphatidyl-D-myo-inositol 3,5-bisphosphate from both L- and D-enantiomers

AUTHOR(S): Han, Fushe; Hayashi, Minoru; Watanabe, Yutaka

CORPORATE SOURCE: Venture Business Laboratory, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: European Journal of Organic Chemistry (2004), (3), 558-566
CODEN: EJOCFK; ISSN: 1434-193X

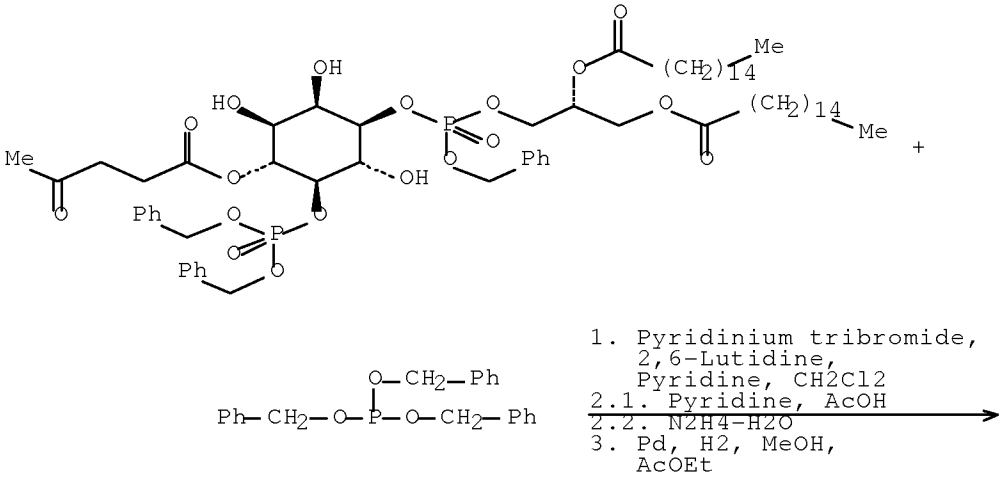
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

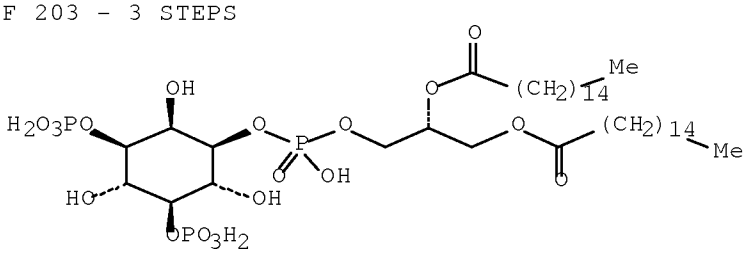
LANGUAGE: English

AB Chem. resoln. of a versatile starting material, 1,2-O-cyclohexylidene-3,4- O-(tetraisopropyldisiloxane-1,3-diyl)-myo-inositol, which is used to access naturally occurring inositol phosphates and phosphatidylinositol phosphates, is described. Starting from both D- and L-enantiomers of the material, the synthesis of phosphatidyl-D-myo-inositol 3,5-bisphosphate [PtdIns(3,5)P2] has been conveniently accomplished via convergent routes. One of the key reactions in the synthetic procedure was the regioselective phosphorylation of suitably protected 1,2,4-triol derivs. of inositol. Phosphorylation of the triol attempted in a 1:12 (volume/volume) pyridine/CH2Cl2 mixture did not proceed at all, whereas in an optimized solvent system, pyridine/CH2Cl2 (1.1:1, volume/volume), the reaction afforded 68% of the desired 1-O-phosphate as a single product. Further investigation by 1H NMR spectroscopy indicated that the reactivity of the three OHs on 1,2,4-triol derivs. is governed by intermol. hydrogen bonding, which may be disrupted by an increase in the proportion of pyridine in the reaction solvent.

RX(80) OF 203 - 3 STEPS



RX(80) OF 203 - 3 STEPS



100%

CON: STEP(1.1) -42 deg C; 15 minutes, -42 deg C; 2 hours, 0 deg C
STEP(2.1) 0 deg C
STEP(2.2) 1.3 hours, 0 deg C -> room temperature
STEP(3) 16 hours, room temperature, 1 atm

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

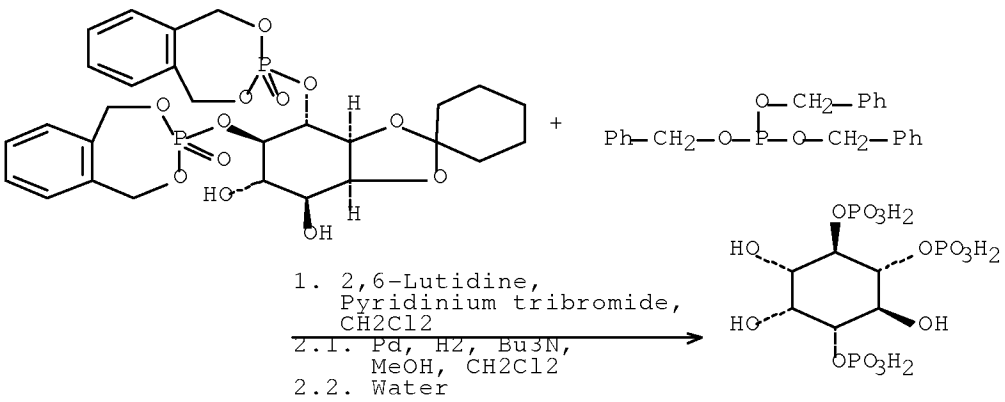
L3 ANSWER 26 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:5254 CASREACT Full-text
TITLE: NBS-DMSO as a nonaqueous non-basic oxidation reagent for the synthesis of oligonucleotides
AUTHOR(S): Uzagare, Matthew C.; Padiya, Kamlesh J.; Salunkhe, Manikrao M.; Sanghvi, Yogesh S.
CORPORATE SOURCE: The Institute of Science, Mumbai, 400 032, India
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(20), 3537-3540
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new method for the oxidn. of nucleoside phosphite triester into phosphate triester under non-basic and nonaq. conditions using NBS-DMSO in CH3CN has been developed. The utility of this method for solution- and solid-phase synthesis of oligonucleotide is demonstrated.

RX(33) OF 49 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 27 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:5236 CASREACT Full-text
TITLE: Regioselective phosphorylation of vicinal 3,4-hydroxy myo-inositol derivative promoted practical synthesis of d-PtdIns(4,5)P2 and D-Ins(1,4,5)P3
AUTHOR(S): Han, Fushe; Hayashi, Minoru; Watanabe, Yutaka
CORPORATE SOURCE: Venture Business Laboratory, Ehime University, Matsuyama, 790-8577, Japan
SOURCE: Tetrahedron (2003), 59(39), 7703-7711
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reactivity of 3 and 4-OH in 3,4-diol myo-inositol derivs. were obsd. through the phosphorylation, acylation and silylation. The results indicated that 3-OH is much more reactive than 4-OH, giving regiospecifically 3-mono-functionalized products. This investigation provided a concise methodol. for the synthesis of natural D-form of PtdIns(4,5)P2 and D-Ins(1,4,5)P3 from L-1,2-O-cyclohexylidene-3,4-O-(tetra- iso-Pr disiloxane-1,3-diyl)-myo-inositol.

RX(21) OF 26 - 2 STEPS



NOTE: 1) regioselective, 2) Na+ and H+cation resin used in last stage
CON: STEP(1.1) -42 deg C; 10 minutes, -42 deg C; 2 hours, 0 deg C
STEP(2) 3 days, room temperature

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 28 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 139:101357 CASREACT Full-text
TITLE: Synthesis of 1-substituted-phytosphingosine: Novel protection of phytosphingosine

AUTHOR(S): Jo, Su Yeon; Kim, Hyoung Cheul; Woo, Seung Woo; Seo, Min Jung; Lee, Gehyeong; Kim, Hyoung Rae

CORPORATE SOURCE: Medicinal Science Division, Korea Research Institute of Chemical Technology, Daejeon, 305-600, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2003), 24(3), 267-268
CODEN: BKCSDE; ISSN: 0253-2964

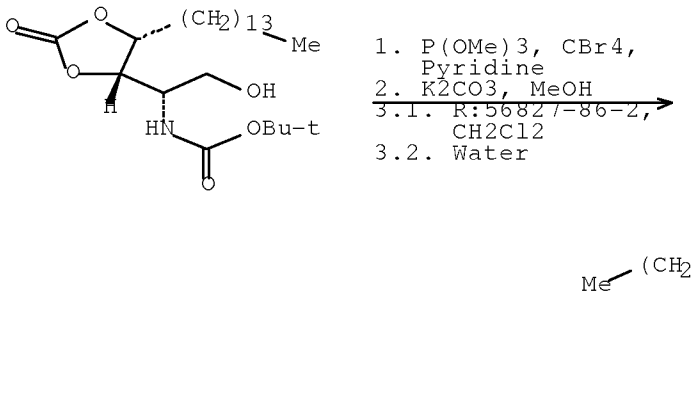
PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Phytosphingosine was protected by the formation of cyclic carbonate in two steps, which could be useful for the derivatizations of 1-position of phytosphingosine. Phytosphingosine-1-phosphate and other derivs. of phytosphingosine were synthesized from the phytosphingosine derivs. protected with cyclic carbonates.

RX(24) OF 26 - 3 STEPS



CON: STEP(1) 0 deg C
STEP(2) 40 deg C
STEP(3.2) 0 deg C

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 29 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:52761 CASREACT Full-text

TITLE: Synthesis of fluorescence-labeled sphingosine and sphingosine 1-phosphate; effective tools for sphingosine and sphingosine 1-phosphate behavior

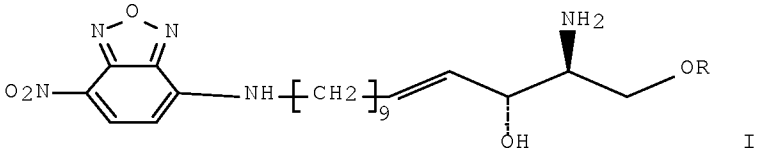
AUTHOR(S): Hakogi, Toshikazu; Shigenari, Toshihiko; Katsumura, Shigeo; Sano, Takamitsu; Kohno, Takayuki; Igarashi, Yasuyuki

CORPORATE SOURCE: School of Science and Technology, Kwansei Gakuin University, Sanda, Hyogo, 669-1337, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(4), 661-664
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

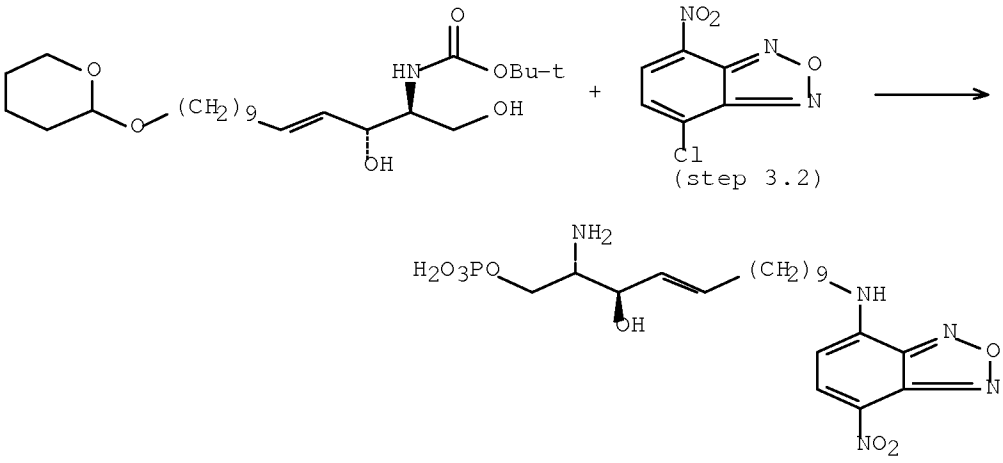
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A fluorescence-labeled sphingosine (I; R = H) and sphingosine 1-phosphate (I; R = PO3H2) have been successfully synthesized from the oxazolidinone Me ester derived from glycidol via monoalkylation and the stereoselective reduction of the resulting ketone. The labeled sphingosine was converted into its phosphate by treatment with sphingosine kinase 1 (SPHK1) from mouse, and in platelets, and it was incorporated into the Chinese Hamster Ovarian (CHO) cells. In addition, MAPK was activated by NBD-Sph-1-P through Edg-1, Sph-1-P receptor.

RX(81) OF 103 - 5 STEPS



(step 3.2)

71%

CON: STEP(2.2) 50 deg C
STEP(3) 60 deg C
STEP(4) -10 deg C

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 30 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 139:36724 CASREACT Full-text
TITLE: Synthesis of (R)-2-methyl-4-deoxy and (R)-2-methyl-4,5-dideoxy analogues of 6-phosphogluconate as potential inhibitors of

6-phosphogluconate dehydrogenase

AUTHOR(S): Dardonville, Christophe; Gilbert, Ian H.

CORPORATE SOURCE: Welsh School of Pharmacy, Cardiff University, Cardiff, CF10 3XF, UK

SOURCE: Organic & Biomolecular Chemistry (2003), 1(3), 552-559
CODEN: OBCRAK; ISSN: 1477-0520

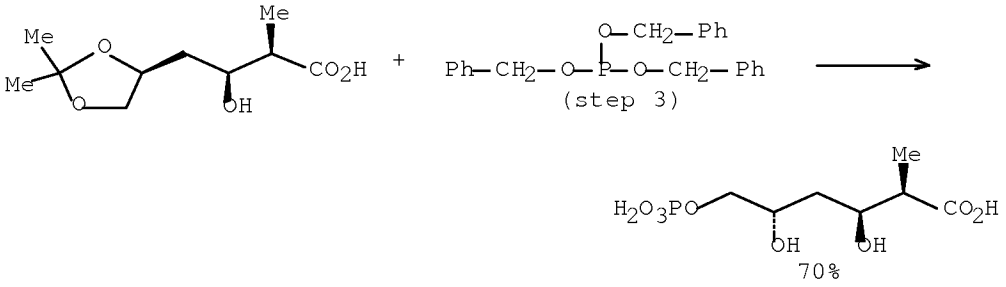
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of (2R)-2-methyl-4,5-dideoxy and (2R)-2-methyl-4-deoxy analogs of 6-phosphogluconate is described. The synthetic strategy relies on the Evans aldol reaction for the installation of the chiral centers in the 2- and 3-positions. The selective phosphorylation at the primary alc. function of (2R,3S)-3,6-dihydroxy-2-methylhexanoic acid benzyl ester and (2R,3S,5S)-3,5,6-trihydroxy-2-methylhexanoic acid benzyl ester was achieved with dibenzyl phosphochloridate and dibenzyl phosphoiodinate resp., working at low temperature (2R,3S)-3-Hydroxy-2-methyl-6- phosphonoxyhexanoic acid was obtained in 25% overall yield from 4-benzyloxybutanol and (2R,3S,5S)-3,5-dihydroxy-2-methyl-6- phosphonoxyhexanoic acid in 10% overall yield from L-malic acid.

RX(121) OF 130 - 5 STEPS



NOTE: 2) stereoselective
CON: STEP(1.1) 16 hours, room temperature
STEP(1.2) room temperature
STEP(2.1) 2 hours, room temperature
STEP(2.2) room temperature
STEP(2.3) room temperature
STEP(2.4) room temperature
STEP(3.1) 30 minutes, -78 deg C; 5 hours, -78 deg C
STEP(4) 24 hours, room temperature
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 2 hours, room temperature

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 31 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:6655 CASREACT Full-text

TITLE: Highly potent inhibitors of TNF-α production. Part I. Discovery of new chemical leads and Their structure-Activity relationships

AUTHOR(S): Matsui, Toshiaki; Kondo, Takashi; Nishita, Yoshitaka; Itadani, Satoshi; Nakatani, Shingo; Omawari, Nagashige; Sakai, Masaru; Nakazawa, Shuichi; Ogata, Akihito; Mori, Hideaki; Terai, Kouichiro; Kamoshima,

Wataru; Ohno, Hiroyuki; Obata, Takaaki; Nakai, Hisao; Toda, Masaaki

CORPORATE SOURCE: Fukui Research Institute, Ono Pharmaceutical Co., Ltd., Sakai, Fukui, 913-8638, Japan

SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(12), 3757-3786
CODEN: BMECEP; ISSN: 0968-0896

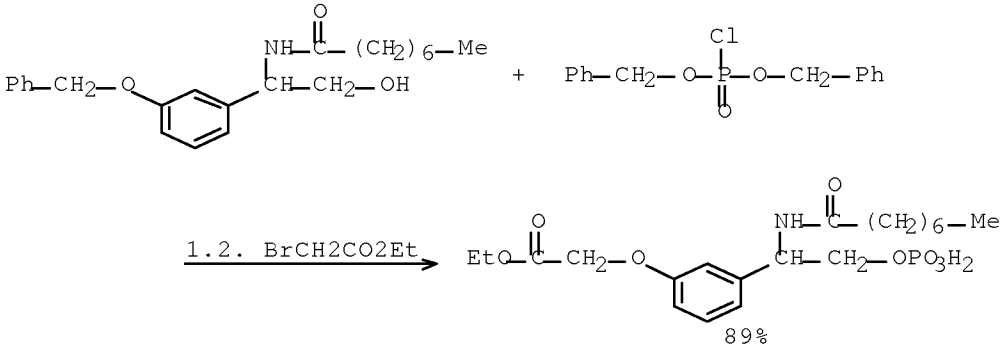
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Discovery of new chem. leads of inhibitors for TNF-α prodn. starting from the chemical modification of 2-(octanoylamino)-2-phenylethyl disodium phosphate (I) is reported. Further biol. studies of I to disclose the site of its action strongly suggested that I inhibits LPS-induced TNF-α expression in the liver and spleen of mice. Structure-activity relationships (SARs) are also discussed and full details including the chemical are reported.

RX(347) OF 529 - 3 STEPS



CON: STEP(1.1) 2 hours, room temperature, 1 atm
STEP(1.2) 2 days, room temperature
STEP(2.1) 3 hours, room temperature
STEP(2.2) 30 minutes, room temperature
STEP(3) 20 hours, room temperature, 1 atm

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 32 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 138:401994 CASREACT Full-text

TITLE: Syntheses of sphingosine-1-phosphate stereoisomers and analogues and their interaction with EDG receptors

AUTHOR(S): Lim, Hyun-Suk; Oh, Yong-Seok; Suh, Pann-Ghill; Chung, Sung-Kee

CORPORATE SOURCE: Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(2), 237-240
CODEN: BMCLE8; ISSN: 0960-894X

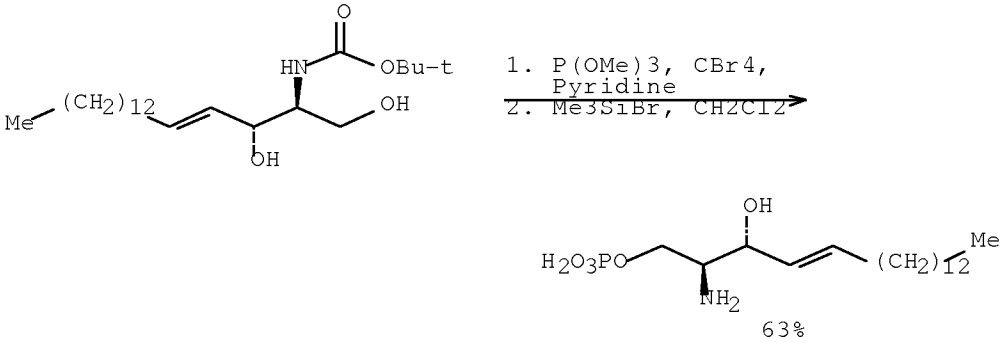
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Sphingosine-1-phosphate (S1P) is considered to be an important regulator of diverse biol. processes acting as a natural ligand to EDG receptors. As a preliminary study to develop potent and selective agonist and antagonist for EDG receptors, we report synthesis of S1P stereoisomers and analogs and their binding affinities to EDG-1, -3, and -5.

RX(18) OF 35 - 2 STEPS



CON: STEP(1) 2 hours
STEP(2) 2 hours

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 33 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 138:369095 CASREACT Full-text

TITLE: A short synthesis of dipalmitoylphosphatidylinositol 4,5-bisphosphate via 3-O-selective phosphorylation of a 3,4-free inositol derivative

AUTHOR(S): Han, Fushe; Hayashi, Minoru; Watanabe, Yutaka

CORPORATE SOURCE: Venture Business Laboratory, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Chemistry Letters (2003), 32(1), 46-47
CODEN: CMLTAG; ISSN: 0366-7022

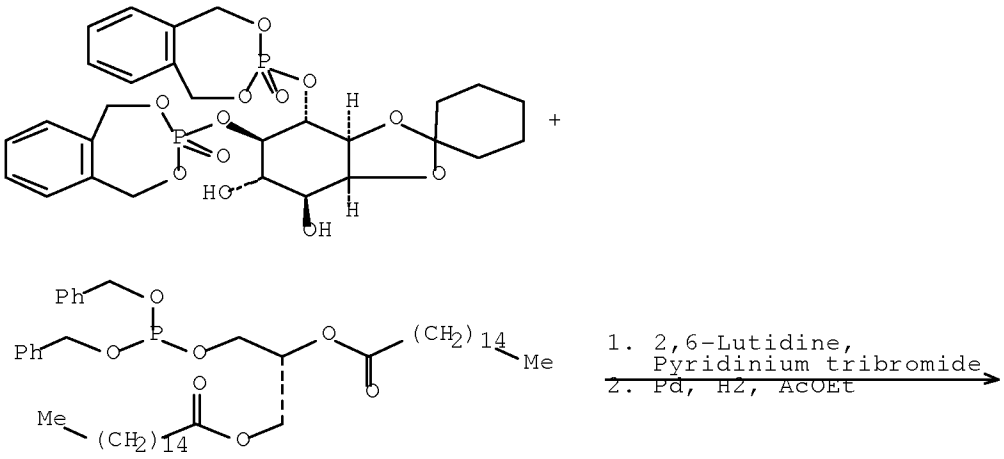
PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

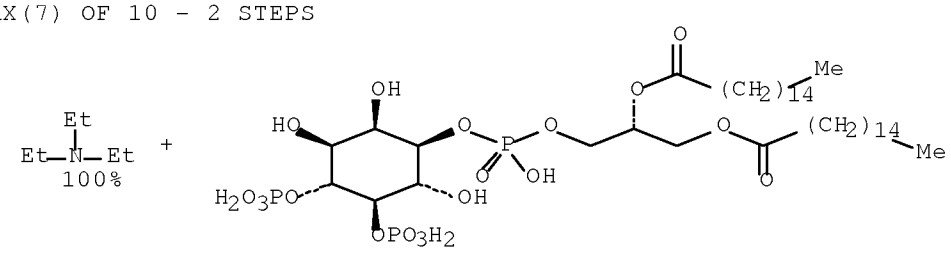
LANGUAGE: English

AB Dipalmitoylphosphatidylinositol 4,5-bisphosphate was conveniently synthesized via the regioselective phosphorylation of L-1,2-O- cyclohexylidene-5,6-di-O-(o-xylylene phosphoryl)-myo-inositol derived from 1,2-O-cyclohexylidene-3,4-O-(tetraisopropyldisiloxane-1,3-diyl)-myo- inositol.

RX(7) OF 10 - 2 STEPS



RX(7) OF 10 - 2 STEPS



CON: STEP(2) 2 days, room temperature

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 34 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 135:284897 CASREACT Full-text

TITLE: Mechanistic Studies on Thiamin Phosphate Synthase: Evidence for a Dissociative Mechanism

AUTHOR(S): Reddick, Jason J.; Nicewonger, Robb; Begley, Tadhg P.

CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, 14853, USA

SOURCE: Biochemistry (2001), 40(34), 10095-10102
CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

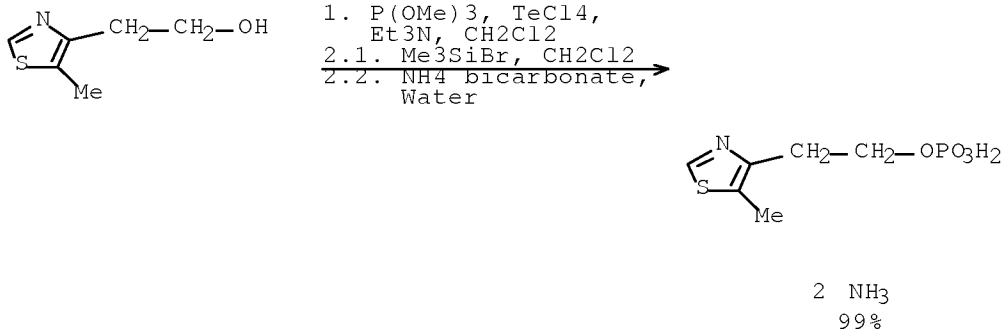
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Thiamin phosphate synthase catalyzes the coupling of 4-methyl-5-(β-hydroxyethyl)thiazole phosphate (Thz-P) and 4-amino-5-(hydroxymethyl)-2-methylpyrimidine pyrophosphate (HMP-PP) to give thiamin phosphate. In this paper, we demonstrate that 4-amino-5-(hydroxymethyl)-2-(trifluoromethyl)pyrimidine pyrophosphate (CF3-HMP-PP) is a very poor substrate [kcat(CH3) > 7800kcat(CF3)] and that 4-amino-5-(hydroxymethyl)-2-methoxypyrimidine pyrophosphate (CH3O-HMP-PP) is a good substrate [kcat(OCH3) > 2.8kcat(CH3)] for the enzyme. We also demonstrate that the enzyme catalyzes positional isotope exchange. These observations are consistent with a

dissociative mechanism (SN1 like) for thiamin phosphate synthase in which the pyrimidine pyrophosphate dissocs. to give a reactive pyrimidine intermediate which is then trapped by the thiazole moiety.

RX(31) OF 49 - 2 STEPS

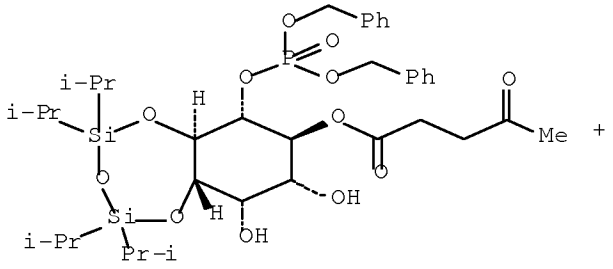


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 35 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 134:86458 CASREACT Full-text
TITLE: Synthesis of dipalmitoyl-phosphatidylinositol 5-phosphate and its modified biological tools
AUTHOR(S): Watanabe, Yutaka; Ishikawa, Hideki
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Ehime University, Matsuyama, 790-8577, Japan
SOURCE: Tetrahedron Letters (2000), 41(44), 8509-8512
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Synthesis of a dipalmitoyl analog of phosphatidylinositol 5-phosphate with the racemic inositol skeleton was achieved via a key intermediate, 1,2-cyclohexylidene-3,4-tetraisopropyldisiloxanyl-myo-inositol. Probes bearing a fluorophore, NBD on a fatty acid chain and a resin for affinity chromatog. were also prepared due to biol. interest in cell division.

RX(12) OF 22 - 2 STEPS



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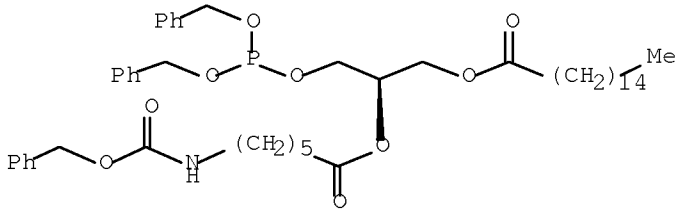
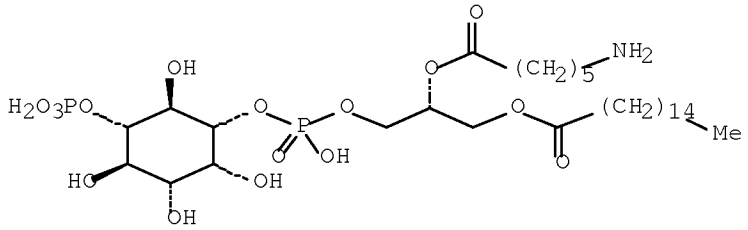


RX(12) OF 22 - 2 STEPS

1. Pyridinium tribromide, 2,6-Lutidine
2.1. N2H4, Pyridine, AcOH
2.2. Pd, H2, t-BuOH, Water
2.3. Bu4N.F, AcOH



NOTE: 1) STEREOSELECTIVE, 2) STEREOSELECTIVE

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 36 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 133:222919 CASREACT Full-text

TITLE: Concise syntheses of L-α-phosphatidyl-D-myo-inositol 3-phosphate (3-PIP), 5-phosphate (5-PIP), and 3,5-bisphosphate (3,5-PIP2)

AUTHOR(S): Falck, J. R.; Krishna, U. Murali; Katipally, Kishta Reddy; Capdevila, Jorge H.; Ulug, Emin T.

CORPORATE SOURCE: Departments of Biochemistry and Pharmacology, University of Texas Southwestern Medical Center, Dallas, TX, 75390, USA

SOURCE: Tetrahedron Letters (2000), 41(22), 4271-4275
CODEN: TELEAY; ISSN: 0040-4039

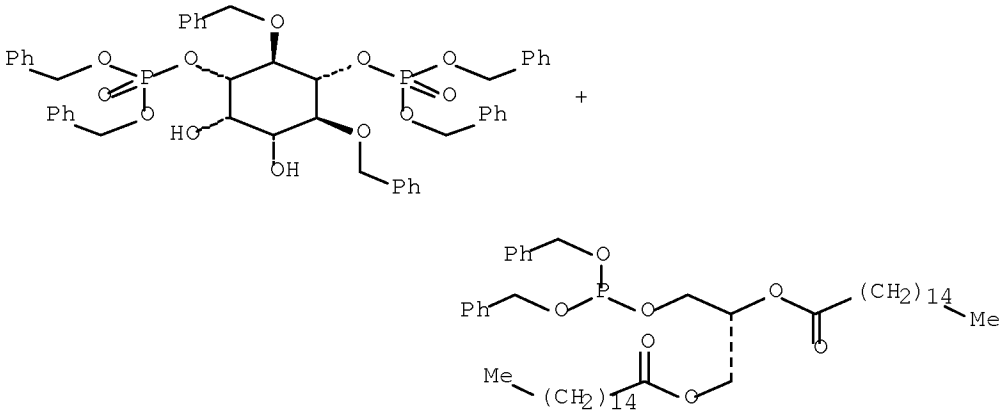
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

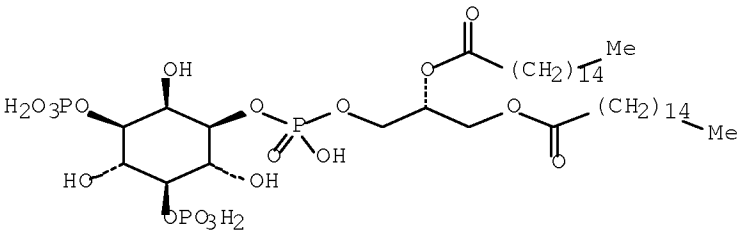
AB Highly efficient, asym. total syntheses of the title phospholipids as well as short-chain and cross-linkable amino ether analogs were achieved in 5-7 steps from a readily available myo-inositol derivative

RX(22) OF 88 - 2 STEPS



RX(22) OF 88 - 2 STEPS

1. Pyridinium tribromide, CH2Cl2, Pyridine, Et3N
2. Pd, H2, NaHCO3, EtOH, Water



79%

NOTE: 1) regioselective

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 37 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

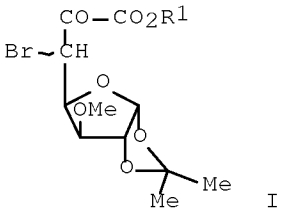
ACCESSION NUMBER: 131:88093 CASREACT Full-text

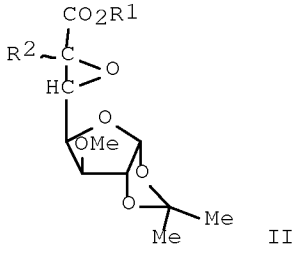
TITLE: Towards a synthesis of glycidic phosphoenol pyruvic acid derivatives

AUTHOR(S): Coutrot, Philippe; Grison, Claude; Tabyaoui, Mohamed; Tabyaoui, Badia; Dumarcay, Stephane

CORPORATE SOURCE: Laboratoire Chimie Organique, Univ. Henri Poincare,

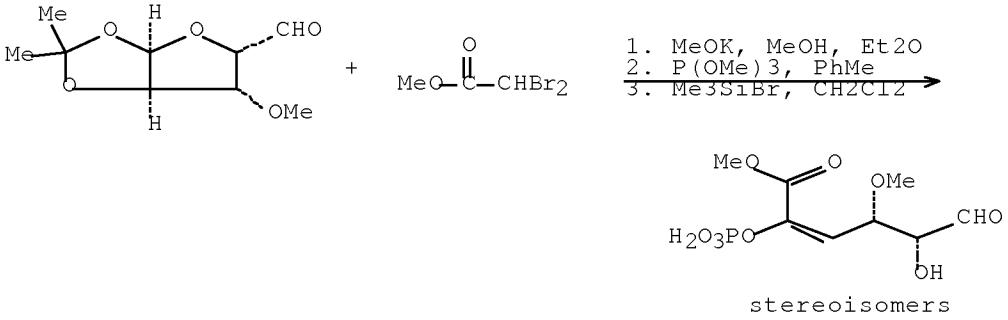
Vandoeuvre-les-Nancy, F-54506, Fr.
SOURCE: Synlett (1999), (6), 792-794
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
GI


I


II

AB Two synthetic routes are proposed to prep. phospho enol pyruvates of xylose as models of potent phosphoenol pyruvate lyase inhibitors: a Perkow reaction between xylose-derived β-bromo α-keto esters I (R1 = Me, CHMe2) and P(OMe)3, and a new reaction between xylose-derived α-bromo glycidates II (R2 = Br, Cl; R1 = Me, CHMe2) and P(OMe)3.

RX(19) OF 23 - 3 STEPS



NOTE: 1) STEREOSELECTIVE, 2) STEREOSELECTIVE, 3) STEREOSELECTIVE

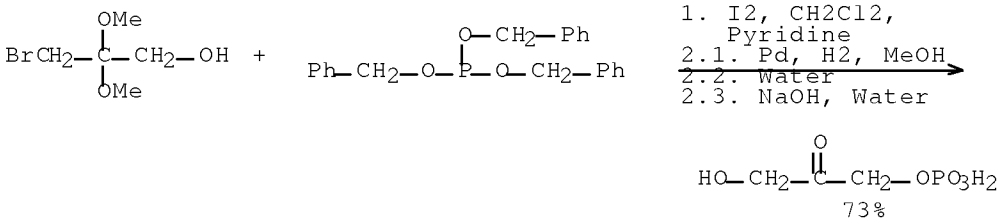
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 38 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 129:276110 CASREACT Full-text
TITLE: Fructose-1,6-bisphosphate aldolase and transketolase: complementary tools for the de novo syntheses of monosaccharides and analogs
AUTHOR(S): Andre, C.; Demuynck, C.; Gefflaut, T.; Guerard, C.; Hecquet, L.; Lemaire, M.; Bolte, J.
CORPORATE SOURCE: UMR 6504 (SEESIB), Departement de Chimie, Universite Blaise Pascal, Aubiere, 63177, Fr.
SOURCE: Journal of Molecular Catalysis B: Enzymatic (1998),

5(1-4), 113-118
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper reports a new synthesis of bromoacetol phosphate and dihydroxyacetone phosphate for use in fructose-1,6-bisphosphate aldolase (FB-aldolase) catalyzed syntheses. Then the activities of FB-aldolase and transketolase towards polyhydroxybutanal analogs of erythrose and erythrose-4-phosphate were studied. These activities were high enough to allow the syntheses of rare heptulose-1-phosphates of the d and l series.

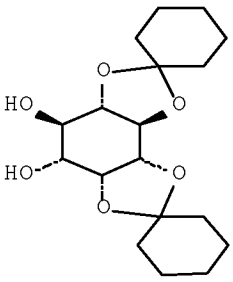
RX(16) OF 29 - 2 STEPS



NOTE: 2) 57% yield over five steps from dibromoacetone
CON: STEP(2.2) 65 deg C

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

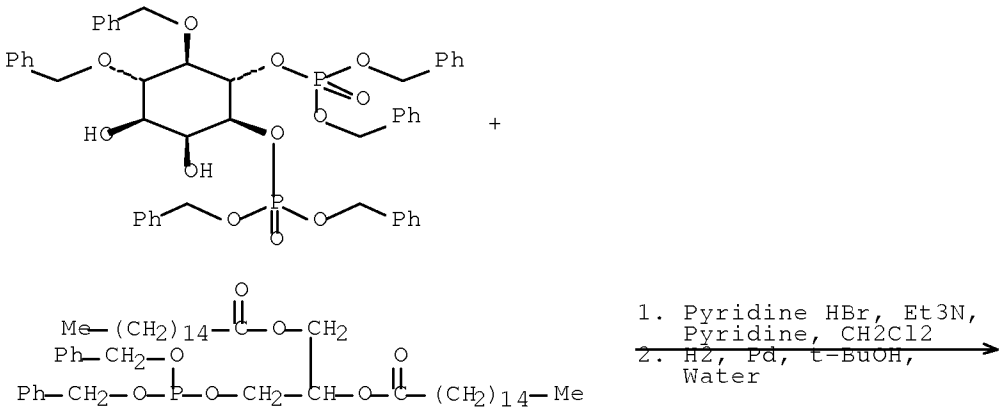
L3 ANSWER 39 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 127:162042 CASREACT Full-text
TITLE: Concise synthesis of L-α-phosphatidyl-D-myo-inositol 3,4-bisphosphate, an intracellular second messenger
AUTHOR(S): Reddy, K. Kishta; Rizo, Josep; Falck, J. R.
CORPORATE SOURCE: Departments Biochemistry and Pharmacology, University Texas Southwestern Medical Center, Dallas, TX, 75235, USA
SOURCE: Tetrahedron Letters (1997), 38(27), 4729-4730
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



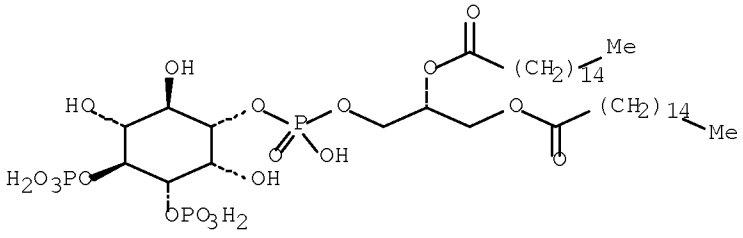
I

AB A highly efficient, asym. total synthesis of the title phospholipid as well as short chain diester and cross-linkable diether analogs was achieved in six steps from the readily available cyclitol I.

RX(7) OF 10 - 2 STEPS



RX(7) OF 10 - 2 STEPS

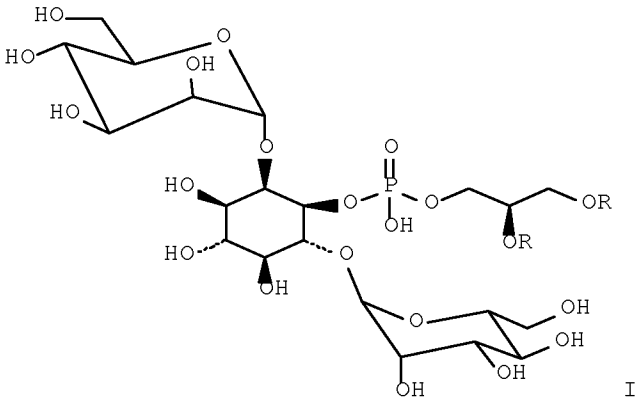


5 Na
96%

NOTE: 1) key step

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

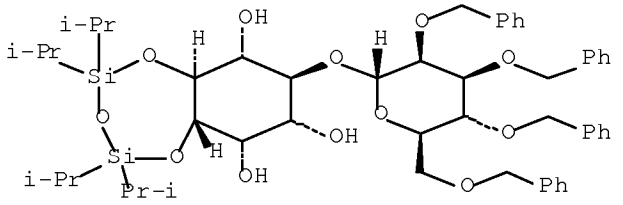
L3 ANSWER 40 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 124:232935 CASREACT Full-text
TITLE: Regiospecific Synthesis of 2,6-Di-O-(α-D-mannopyranosyl)phosphatidyl-D-myo-inositol
AUTHOR(S): Watanabe, Yutaka; Yamamoto, Takashi; Ozaki, Shoichiro
CORPORATE SOURCE: Faculty of Engineering, Ehime University, Matsuyama, 790, Japan
SOURCE: Journal of Organic Chemistry (1996), 61(1), 14-15
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

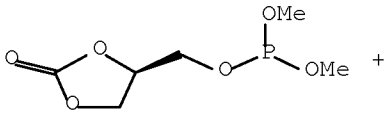
AB A concise synthesis of 2,6-di-O-α-D-mannopyranosylphosphatidyl-D-myo- inositol I [R = CO(CH2)16Me] has been accomplished by completely regioselective introduction of the requisite substituents on myo-inositol. The pivotal intermediate, 1,2-O-cyclohexylidene-3,4-O- (tetraisopropyldisiloxane-1,3-diyl)-myo-inositol, was glycoylated regioselectively at the 6-position using a mannopyranosyl phosphite as the glycosyl donor. After removing the cyclohexylidene group, the resultant 1,2-diol derivative was phosphorylated by the reaction with a glycerol phosphite in the presence of pyridinium bromide perbromide to afford regioselectively 1-O-phosphate. This was then glycosylated regio- and stereoselectively at the 2-position by the phosphite approach as above. The 1,2-O-carbonyl protecting group in the glycerol moiety was removed by the reaction with the ethylmagnesium chloride without the migration of the phosphite function, and the resulting diol was acylated and finally deprotected.

RX(27) OF 29 - 5 STEPS



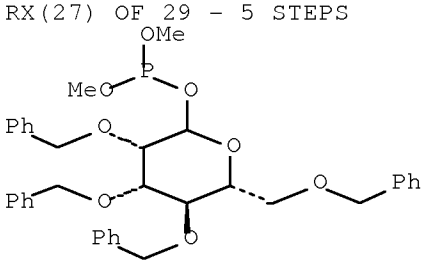
stereoisomers

+



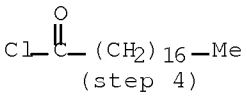
+

RX(27) OF 29 - 5 STEPS

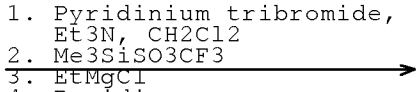


(step 2)

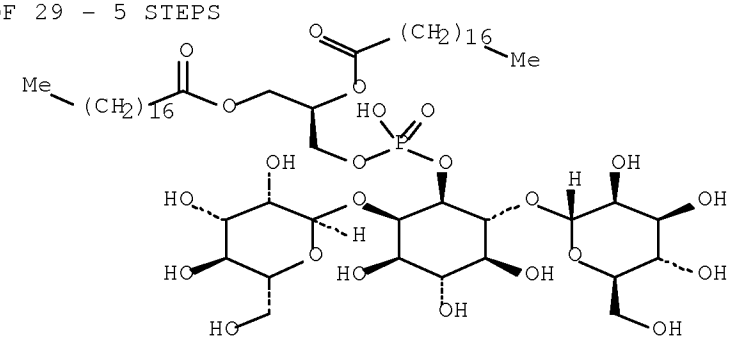
+



(step 4)



RX(27) OF 29 - 5 STEPS



stereoisomers

NOTE: 1) 83% overall, regioselective, 4) 73% OVERALL, 5) ISOMERIC REACTANTS ALSO PRESENT

L3 ANSWER 41 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 109:110765 CASREACT Full-text

TITLE: Synthesis of C-arabinofuranosyl compounds. Phosphonate and carboxylate isosteres of D-arabinose 1,5-bisphosphate

AUTHOR(S): Maryanoff, Bruce E.; Nortey, Samuel O.; Inners, Ruth R.; Campbell, Susan A.; Reitz, Allen B.; Liotta, Dennis

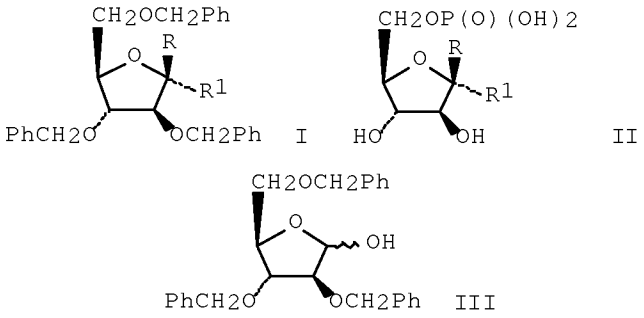
CORPORATE SOURCE: Chem. Res. Dep., McNeil Pharm., Spring House, PA, 19477, USA

SOURCE: Carbohydrate Research (1987), 171, 259-78
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

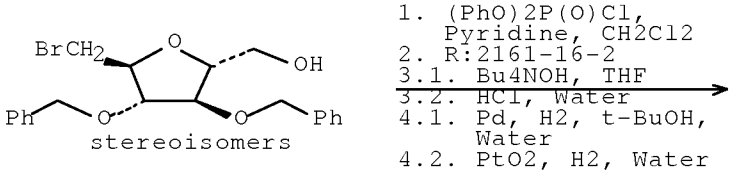
LANGUAGE: English

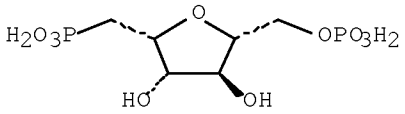
GI



AB Electrophile-mediated cyclization. of 3,4,6-tri-O-benzyl-1,2-dideoxy-D-arabino-hex-1-enitol with N-bromosuccinimide yielded primarily 2,5-anhydro-3,4,6-tri-O-benzyl-1-bromo-1-deoxy-D-glucitol (I; R = CH2Br, R1 = H). This apparently kinetically controlled reaction was of key importance in the successful synthesis of a phosphonate analog of β-D-arabinose 1,5-bisphosphate [II; R = OP(O)(OH)2, R1 = H], namely, 2,5-anhydro-1-deoxy-1-phosphono-D-glucitol 6-phosphate [II; R = CH2OP(O)(OH2), R1 = H] with high stereoselectivity. By contrast, condensation of the sodium salt of tetra-Et methylenediphosphonate and 2,3,5-tri-O-benzyl-D-arabinose (III) gave a phosphonate compound slightly enriched in the 2,5-anhydro-D-mannitol (α) isomer. In the Wittig-Michael reaction of stabilized phosphoranes with (III), the α isomer preponderated. Since equilibration of Me 3,6-anhydro-4,5,7-tri-O- benzyl-2-deoxy-D-glycero-D-galacto- (I; R = H, R1 = CH2O2Me) and -D-gulo-heptonate (I; R = CH2CO2Me, R1 = H) (5:1) resulted in a 1:1 α:β ratio, the preference for the 2,5-anhydro-D-mannitol (α) isomer probably reflects a kinetic bias. The carbomethoxy anomers were converted independently into the α and β carboxylate isosteres [II (R = H, R1 = CH2CO2H; R = CH2CO2H, R1 = H), resp.] of D-arabinose 1,5-diphosphate. Empirical force field calcns. (MMP2) and NMR expts. were conducted on the pairs of diastereomers I (R = H, R1 = CH2Br; R = CH2Br, R1 = H; and R = H, R1 = CH2CO2Me; R = CH2CO2Me, R1 = H). The calcns. predict that the α and β anomers of each pair have similar energies, differing by only 2.1 kJ/mol. Compds. II [R = CH2P(O)(OH)2, CH2CO2H, R1 = H; R = H, R1 = CH2CO2H] were evaluated for biol. activity.

RX(71) OF 140 - 4 STEPS





NOTE: 1) 67% overall, 2) 16 h, 178.degree.

L3 ANSWER 42 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 104:225103 CASREACT Full-text

TITLE: Stereoselectivity in the electrophile-promoted cyclizations of a hydroxyolefin derived from arabinose. Synthesis of a phosphonate isostere of β-D-arabinose-1,5-diphosphate

AUTHOR(S): Reitz, Allen B.; Nortey, Samuel O.; Maryanoff, Bruce E.

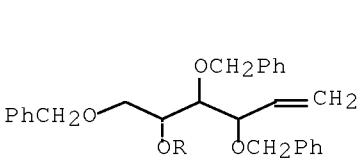
CORPORATE SOURCE: Chem. Res. Dep., McNeil Pharm., Spring House, PA, 19477, USA

SOURCE: Tetrahedron Letters (1985), 26(33), 3915-18
CODEN: TELEAY; ISSN: 0040-4039

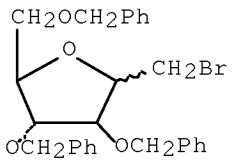
DOCUMENT TYPE: Journal

LANGUAGE: English

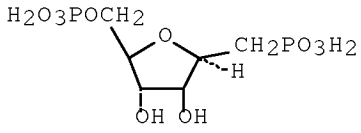
GI



I



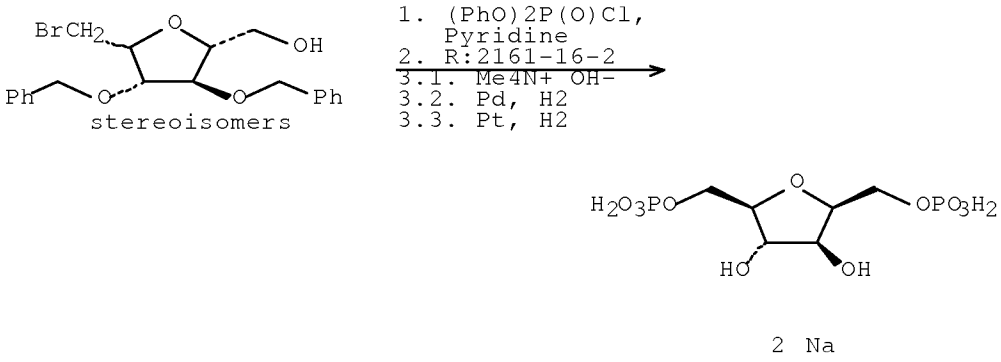
II



III

AB Cyclization of hydroxyolefin I [R = H, SiMe2CMe3, CH2O(CH2)2SiMe3] with NBS or Hg(OAc)2 yielded predominantly the β isomer of a C-arabinofuranoside II. II was acetylated, phosphorylated and hydrolyzed to yield isostere III.

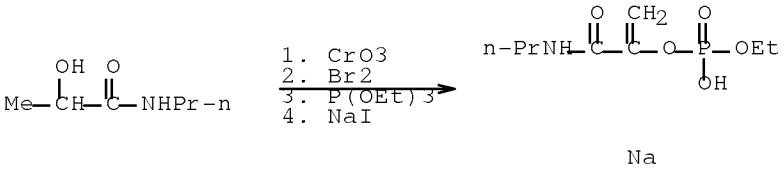
RX(36) OF 50 - 3 STEPS



L3 ANSWER 43 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 101:37906 CASREACT Full-text
TITLE: Phosphoenol pyruvamides. Amide-phosphate interactions in analogs of phosphoenol pyruvate
AUTHOR(S): Kluger, Ronald; Chow, Jane Frances; Croke, James J.
CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.
SOURCE: Journal of the American Chemical Society (1984), 106(14), 4017-20
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB CH2:C[OP(O)(OR)2]CONHR1 (I; R = Et, R1 = Pr, Ph) were obtained in the reaction of (EtO)3P with BrCH2COCONHR1. The 1st order hydrolysis kinetics, of the Et ester portion, of I are 4 orders of magnitude faster than that estimated for (EtO)3P (under comparable conditions) indicating neighboring participation by the carboxamide group. The Et group in I is cleaved much more slowly than that in unconjugated enol phosphate monoesters indicating that the I hydrolysis mechanism involves amide addition to the adjacent phosphate to form a reactive cyclic intermediate. The implication of I hydrolysis for phosphoenol pyruvate studies in enzyme systems and for peptide-nucleotide interactions are discussed.

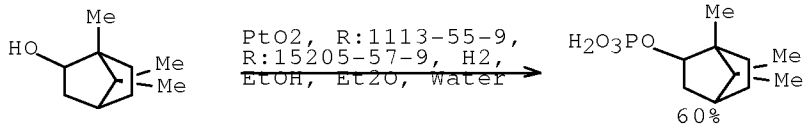
RX(25) OF 26 - 4 STEPS



L3 ANSWER 44 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 60:61195 CASREACT Full-text
TITLE: Synthesis of testosterone dimethyl phosphate, bornyl phosphate, and adenosine 5'-phosphate
AUTHOR(S): Hata, Tsujiaki; Mukaiyama, Teruaki
CORPORATE SOURCE: Tokyo Inst. Technol.

SOURCE: Bulletin of the Chemical Society of Japan (1964), 37(1), 103-4
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB (MeO)3P added to a soln. of 1 mole testosterone and 1 mole NCCHBrCONH2 (I) in dry ether at -40° gave 62% testosterone di-Me phosphate (II). Borneol with I and (PhCH2O)3P, followed by hydrogenolysis to remove the benzyl group, gave 60% bornyl phosphate (III). 2',3'-O- Isopropylideneadenosine (1 mole) treated with 1 mole NCCHBrCONH2 and 1 mole (PhCH2O)3P, followed by hydrogenolysis and hydrolysis gave 62% adenosine 5'-phosphate.

RX(1) OF 2



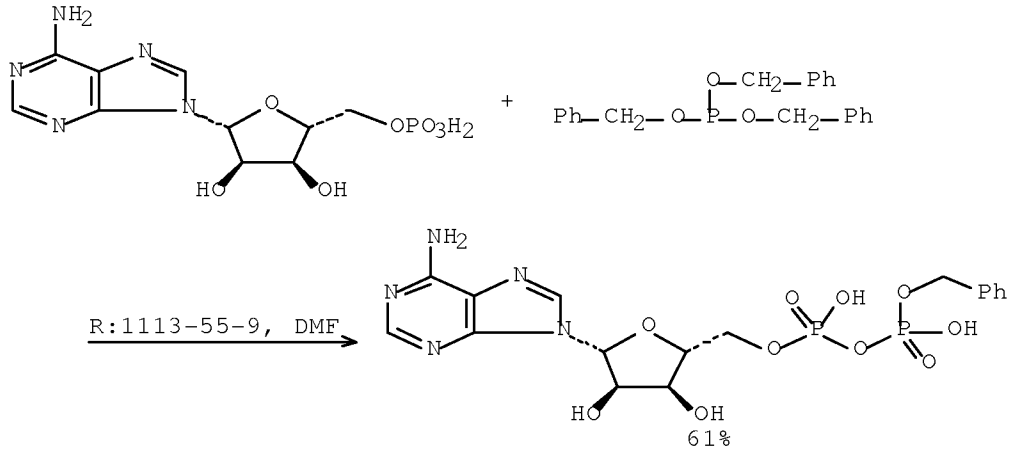
NOTE: Classification: O-Phosphorisation; Hydrogenolysiscatalysis; Oxidation; # Conditions: H2NCOCHBrCN; (PhCH2O)3P; Et2O 20 deg; 2h 20 deg overnight; H2/PtO2 EtOH H2O

L3 ANSWER 45 OF 45 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 60:15998 CASREACT Full-text
TITLE: Pyrophosphates
INVENTOR(S): Mukaiyama, Teruaki; Hata, Tsujiaki
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 38017308	B4	19630906	JP	19620331
DE 1200819			DE	
FR 1372445			FR	
GB 1007770			GB	
US 3188310		19650608	US 1963-269719	19630401
PRIORITY APPLN. INFO.:			JP	19620331

AB A mixt. of 1.54 g. diethyl phosphite and 1.63 g. α- monobromocyanoacetamide in 150 ml. Et2O is kept at -50°, a solution of 1.24 g. trimethyl phosphate in 15 ml. Et2O gradually added, the mixture allowed to stand 2 hrs. and filtered, and the filtrate distilled in vacuo to give 2.4 g. dimethyl diethyl pyrophosphate, b0.004 100-6°. Similarly prepared are tetraethyl pyrophosphate (b1 135-6°), diethyl dibutyl pyrophosphate (b0.02 114-18°), bis(p-nitrophenyl) N-cyclohexylphosphamidate (m. 172-3°), and monobenzyl 5'-adenosine diphosphate.

RX(2) OF 2



61%

NOTE: Classification: Phosphorylation; Condensation; # Conditions: H2NCOCH(Br)CN; BuNH2 DMF; 6h; 20 deg 24h

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	340.99	341.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-33.75	-33.75

STN INTERNATIONAL LOGOFF AT 16:25:52 ON 14 JUL 2008